

Clustering using skewed multivariate heavy tailed distributions with flexible tail behaviour

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Abstract

The family of location and scale mixtures of Gaussians has the ability to generate a number of flexible distributional forms. It nests as particular cases several important asymmetric distributions like the Generalised Hyperbolic distribution. The Generalised Hyperbolic distribution in turn nests many other well known distributions such as the Normal Inverse Gaussian (NIG) whose practical relevance has been widely documented in the literature. In a multivariate setting, we propose to extend the standard location and scale mixture concept into a so called multiple scaled framework which has the advantage of allowing different tail and skewness behaviours in each dimension of the variable space with arbitrary correlation between dimensions. Estimation of the parameters is provided via an EM algorithm with a particular focus on NIG distributions. Inference is then extended to cover the case of mixtures of such multiple scaled distributions for application to clustering. Assessments on simulated and real data confirm the gain in degrees of freedom and flexibility in modelling data of varying tail behaviour and directional shape.

1 Introduction

A popular approach to identify groups or clusters within data is via a parametric finite mixture model (Fruwirth-Schnatter, 2006). While the vast majority of work on such mixtures has been based on Gaussian mixture models (see *e.g.* Fraley and Raftery, 2002). in many applications the tails of Gaussian distributions are shorter than appropriate and the Gaussian shape is not suitable for highly asymmetric data. A natural extension to the Gaussian case is to consider families of distributions which can be represented as *location and scale Gaussian mixtures* of the form,

$$p(\mathbf{y}; \boldsymbol{\mu}, \boldsymbol{\Sigma}, \boldsymbol{\beta}, \boldsymbol{\theta}) = \int_0^\infty \mathcal{N}_M(\mathbf{y}; \boldsymbol{\mu} + w\boldsymbol{\beta}\boldsymbol{\Sigma}, w\boldsymbol{\Sigma}) f_W(w; \boldsymbol{\theta}) dw, \quad (1)$$

where $\mathcal{N}_M(\cdot; \boldsymbol{\mu} + w\boldsymbol{\beta}\boldsymbol{\Sigma}, w\boldsymbol{\Sigma})$ denotes the M -dimensional Gaussian distribution with mean $\boldsymbol{\mu} + w\boldsymbol{\beta}\boldsymbol{\Sigma}$ and covariance $w\boldsymbol{\Sigma}$ and f_W is the probability distribution

of a univariate positive variable W referred to hereafter as the weight variable. The parameter β is an additional M -dimensional vector parameter for skewness. When $\beta = 0$ and W^{-1} follows a Gamma distribution $\mathcal{G}(\nu/2, \nu/2)$ ¹ i.e. f_W is an Inverse Gamma distribution $inv\mathcal{G}(\nu/2, \nu/2)$ where ν denotes the degrees of freedom, we recover the well known multivariate t -distribution (Kotz and Nadarajah, 2004). The weight variable W in this case effectively acts to govern the tail behaviour of the distributional form from light tails ($\nu \rightarrow \infty$) to heavy tails ($\nu \rightarrow 0$) depending on the value of ν (a form of robust tuning parameter).

In the more general case of, for example, allowing $\beta \neq 0$ and f_W being a Generalised Inverse Gaussian (GIG) distribution, we recover the family of Generalised Hyperbolic (GH) distributions (Barndorff-Nielsen, 1997) which is able to represent a particularly large number of distributional forms. The GIG distribution depends on three parameters and is given by

$$\begin{aligned} f_W(w; \lambda, \gamma, \delta) &= \mathcal{GIG}(w; \lambda, \gamma, \delta) \\ &= \left(\frac{\gamma}{\delta}\right)^\lambda \frac{w^{\lambda-1}}{2K_\lambda(\delta\gamma)} \exp\left(-\frac{1}{2}(\delta^2/w + \gamma^2 w)\right), \end{aligned} \quad (2)$$

where $K_r(x)$ is the modified Bessel function of the third kind of order r evaluated at x ². Depending on the parameter choice for the GIG, special cases of the GH family include: the multivariate GH distribution with hyperbolic margins ($\lambda = 1$) (Schmidt et al., 2006); the Normal Inverse Gaussian ($\lambda = -1/2$) distribution (Barndorff-Nielsen et al., 1982); the multivariate hyperbolic ($\lambda = \frac{M+1}{2}$) distribution (Barndorff-Nielsen, 1977); the hyperboloid ($\lambda = 0$) distribution (Jensen, 1981); the hyperbolic skew- t ($\lambda = -\nu, \gamma = 0$) distribution (Aas et al., 2005); and the Normal Gamma ($\lambda > 0, \mu = 0, \delta = 0$) distribution (Griffin and Brown, 2010) amongst others. For applied problems, the most popular of these forms appears to be the Normal Inverse Gaussian (NIG) distribution (Barndorff-Nielsen et al., 1982; Protassov, 2004; Karlis and Santourian, 2009). It has been used extensively in financial applications, see Protassov (2004); Barndorff-Nielsen (1997) or Aas et al. (2005); Aas and Hobaek Haff (2006) and references therein, but also in geoscience and signal processing (Gjerde et al., 2011; Oigard et al., 2004). Another popular distributional form allowing for skewness and heavy or light tails includes different forms of the multivariate skew- t like the proposals of Sahu et al. (2003); Lee and McLachlan (2012); Lin (2010) for skew- t distributions where skewness and covariance are separated and Azzalini and Dalla Valle (1996); Basso et al. (2010); Pyne et al. (2009) for other formulations that do not share this separation property. Most of these distributional forms are also able to be represented as *location and scale Gaussian mixtures*.

Although the above approaches provide for great flexibility in modelling data of highly asymmetric and heavy tailed form, they assume f_W to be a univariate distribution and hence each dimension is governed by the same amount of tailweight. There have been various approaches to address this issue in the statistics literature for both symmetric and asymmetric distributional forms. In his work, Jones (2002) proposes a dependent bivariate t -distribution with

¹The Gamma probability density function is $\mathcal{G}(w; \alpha, \beta) = \beta^\alpha \Gamma(\alpha)^{-1} w^{\alpha-1} \exp(-\beta w)$

²The modified Bessel function (see Appendix in Jorgensen (1982)) is $K_r(x) = 1/2 \int_0^\infty y^{r-1} \exp(-\frac{1}{2}x(y + y^{-1})) dy$

marginals of different degrees of freedom but the tractability of the extension to the multivariate case is unclear. Other distributions have been presented in chapters 4 and 5 of Kotz and Nadarajah (2004) but their formulations tend to be appreciably more complicated, often already in the expression of their probability density function. Increasingly, there has been much research on copula approaches to account for flexible distributional forms but the choice as to which one to use in this case and the applicability to (even) moderate dimensions is also not clear (Daul et al., 2003; Giordani et al., 2008; Demarta and McNeil, 2005). In general the papers take various approaches whose relationships have been characterized in the bivariate case by Shaw and Lee (2008). However, most of these approaches suffer either from the non-existence of a closed-form pdf or from a difficult generalization to more than two dimensions. An alternative approach (Schmidt et al., 2006), which takes advantage of the property that Generalised Hyperbolic distributions are closed under affine-linear transformations, derives independent GH marginals but estimation of parameters appears to be restricted to density estimation, and not formally generalisable to estimation settings for a broad range of applications (*e.g.* clustering, regression, *etc.*). A more general approach outside of the GH distribution setting is outlined in (Ferreira and Steel, 2007b,a) with a particular focus on regression models using a Bayesian framework.

In this paper, we show that the location and scale mixture representation can be further explored and propose a so-called *multiple scaled* framework that is considerably simpler than those previously proposed with distributions exhibiting interesting properties. The approach builds upon, and develops further, previous work on scale mixture of Gaussians (Forbes and Wraith, 2013) where the focus was on *symmetric* multiple scaled heavy tailed distributions. In this paper, we consider the more general case of including location in addition to scale in the multiplied scaled framework. This generalisation provides a much wider variety of distributional forms, allowing different tail and skewness behavior in each dimension of the variable space with arbitrary correlation between dimensions. The key elements of the approach are similar to that in Forbes and Wraith (2013). The introduction of multidimensional weights and a decomposition of the matrix Σ in (1) is used to facilitate estimation and also allows for arbitrary correlation between dimensions. This principle was illustrated in the Supplementary Materials (one-page Appendix B) of Forbes and Wraith (2013) with the example of the NIG distribution. However, no details were given on the properties, estimation and application of these new location and scale representations. The content of this paper is therefore entirely new. Using the Generalised Hyperbolic distribution as an example, we present the more general case of multiple scaled Generalised Hyperbolic distributions for which we provide a number of properties in Sections 2.2 to 2.4.

The paper is outlined as follows. In Section 2, further details of the GH distribution and the particular case of the NIG distribution are briefly outlined, followed by details of the proposed new family of multiple scaled GH (and NIG) distributions. In Section 3, we outline an approach for maximum likelihood estimation of the parameters for the multiple scaled NIG distribution via the EM algorithm. In Section 4 we explore the performance of the approach on several simulated and real data sets in the context of clustering. Section 5 concludes with a discussion and areas for further research.

2 Multiple scaled Generalised Hyperbolic distributions

In this section we outline further details of the standard (single weight) multivariate GH distribution (Sect. 2.1) and then the proposed multiple scaled GH distribution (Sect. 2.2 to 2.4). As the NIG distribution appears to be the most popular case of the GH family in applications we also outline further details of this distribution and its multiple scaled form which will be used in Section 4 to assess the performance on simulated and real datasets.

2.1 Multivariate Generalised Hyperbolic distribution

As mentioned previously the Generalised Hyperbolic distribution can be represented in terms of a *location and scale Gaussian mixture*. In the statistics literature, the representation is also often referred to as a normal mean-variance mixture. Using notation equivalent to that of Barndorff-Nielsen (1997) Section 7 and Protasov (2004), the multivariate GH density takes the following form

$$\begin{aligned}
 p(\mathbf{y}; \boldsymbol{\mu}, \boldsymbol{\Sigma}, \boldsymbol{\beta}, \lambda, \gamma, \delta) &= \mathcal{GH}(\mathbf{y}; \boldsymbol{\mu}, \boldsymbol{\Sigma}, \boldsymbol{\beta}, \lambda, \gamma, \delta) \\
 &= \int_0^\infty \mathcal{N}_M(\mathbf{y}; \boldsymbol{\mu} + w\boldsymbol{\Sigma}\boldsymbol{\beta}, w\boldsymbol{\Sigma}) \mathcal{GIG}(w; \lambda, \gamma, \delta) dw \\
 &= (2\pi)^{-M/2} |\boldsymbol{\Sigma}|^{-1/2} \left(\frac{\gamma}{\delta}\right)^\lambda \left(\frac{q(\mathbf{y})}{\alpha}\right)^{\lambda - \frac{M}{2}} K_{\lambda - \frac{M}{2}}(q(\mathbf{y})\alpha) \\
 &\quad \times (K_\lambda(\delta\gamma))^{-1} \exp(\boldsymbol{\beta}^T(\mathbf{y} - \boldsymbol{\mu}))
 \end{aligned} \tag{3}$$

where $|\boldsymbol{\Sigma}|$ denotes the determinant of $\boldsymbol{\Sigma}$, $\delta > 0$, and $q(\mathbf{y})$ and α are given by

$$q(\mathbf{y})^2 = \delta^2 + (\mathbf{y} - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} (\mathbf{y} - \boldsymbol{\mu}), \tag{4}$$

$$\gamma^2 = \alpha^2 - \boldsymbol{\beta}^T \boldsymbol{\Sigma} \boldsymbol{\beta} \geq 0. \tag{5}$$

The parameters $\boldsymbol{\beta}$ and $\boldsymbol{\mu}$ are column vectors of length M ($M \times 1$ vector).

An alternative (hierarchical) representation of the multivariate GH distribution (which is useful for simulation) can be seen as,

$$\begin{aligned}
 \mathbf{Y}|W = w &\sim \mathcal{N}_M(\boldsymbol{\mu} + w\boldsymbol{\Sigma}\boldsymbol{\beta}, w\boldsymbol{\Sigma}) \\
 W &\sim \mathcal{GIG}(\lambda, \gamma, \delta)
 \end{aligned} \tag{6}$$

By setting $\lambda = -1/2$ in the GIG distribution we recover the Inverse Gaussian (IG) distribution,

$$f_W(w; \gamma, \delta) = \mathcal{IG}(w; \gamma, \delta) \tag{7}$$

$$= \frac{\delta}{w^{3/2} \sqrt{2\pi}} \exp(\delta\gamma) \exp\left(-\frac{1}{2}(\delta^2/w + \gamma^2 w)\right) \tag{8}$$

which (when used as the mixing distribution) leads to the NIG distribution

$$\begin{aligned}
 p(\mathbf{y}; \boldsymbol{\mu}, \boldsymbol{\Sigma}, \boldsymbol{\beta}, \gamma, \delta) &= \mathcal{NIG}(\mathbf{y}; \boldsymbol{\mu}, \boldsymbol{\Sigma}, \boldsymbol{\beta}, \gamma, \delta) \\
 &= \int_0^\infty \mathcal{N}_M(\mathbf{y}; \boldsymbol{\mu} + w\boldsymbol{\Sigma}\boldsymbol{\beta}, w\boldsymbol{\Sigma}) \mathcal{IG}(w; \gamma, \delta) dw \\
 &= \frac{\delta}{2^{\frac{M-1}{2}}} \exp(\delta\gamma + (\mathbf{y} - \boldsymbol{\mu})^T \boldsymbol{\beta}) \left(\frac{\alpha}{\pi q(\mathbf{y})}\right)^{\frac{M+1}{2}} K_{\frac{M+1}{2}}(\alpha q(\mathbf{y}))
 \end{aligned}$$

where α and q are defined as in definitions (5) and (4).

Using the parameterisation of (Barndorff-Nielsen, 1997), an identification problem arises as the distributions $\mathcal{GH}(\boldsymbol{\mu}, \boldsymbol{\Sigma}, \boldsymbol{\beta}, \lambda, \gamma, \delta)$ and $\mathcal{GH}(\boldsymbol{\mu}, k^2\boldsymbol{\Sigma}, \boldsymbol{\beta}, \lambda, k\gamma, \delta/k)$ are identical for any $k > 0$. For the estimation of parameters, this problem can be solved by constraining the determinant of $\boldsymbol{\Sigma}$ to be 1.

2.2 Multiple Scaled Generalised Hyperbolic distribution (MSGH)

As mentioned in the Introduction, most of the work on multivariate *location and scale mixture of Gaussians* has focused on studying different choices for the weight distribution f_W (see *e.g.* Eltoft et al., 2006). Surprisingly, little work to our knowledge has focused on the dimension of the weight variable W which in most cases has been considered as univariate. The difficulty in considering multiple weights is the interpretation of such a multidimensional case. The extension we propose consists then of introducing the parameterization of the scale matrix into $\boldsymbol{\Sigma} = \boldsymbol{D}\boldsymbol{A}\boldsymbol{D}^T$, where \boldsymbol{D} is the matrix of eigenvectors of $\boldsymbol{\Sigma}$ and \boldsymbol{A} is a diagonal matrix with the corresponding eigenvalues of $\boldsymbol{\Sigma}$. The matrix \boldsymbol{D} determines the orientation of the Gaussian and \boldsymbol{A} its shape. Such a parameterization has the advantage to allow an intuitive incorporation of the multiple weight parameters. We propose to set the scaled covariance in (1) to $\boldsymbol{D}\boldsymbol{\Delta}_w\boldsymbol{A}\boldsymbol{D}^T$, where $\boldsymbol{\Delta}_w = \text{diag}(w_1, \dots, w_M)$ is the $M \times M$ diagonal matrix whose diagonal components are the weights $\{w_1, \dots, w_M\}$. The generalization we propose is therefore to define

$$p(\mathbf{y}; \boldsymbol{\mu}, \boldsymbol{D}, \boldsymbol{A}, \boldsymbol{\beta}, \boldsymbol{\theta}) = \int_0^\infty \dots \int_0^\infty \mathcal{N}_M(\mathbf{y}; \boldsymbol{\mu} + \boldsymbol{D}\boldsymbol{\Delta}_w\boldsymbol{A}\boldsymbol{D}^T\boldsymbol{\beta}, \boldsymbol{D}\boldsymbol{\Delta}_w\boldsymbol{A}\boldsymbol{D}^T) \times f_w(w_1 \dots w_M; \boldsymbol{\theta}) dw_1 \dots dw_M, \quad (9)$$

where $\boldsymbol{\Delta}_w = \text{diag}(w_1, \dots, w_M)$, and the weights are assumed to be independent *i.e.* $f_w(w_1 \dots, w_M; \boldsymbol{\theta}) = f_{W_1}(w_1; \boldsymbol{\theta}_1) \dots f_{W_M}(w_M; \boldsymbol{\theta}_M)$. Equation (9) can be equivalently written as

$$p(\mathbf{y}; \boldsymbol{\mu}, \boldsymbol{D}, \boldsymbol{A}, \boldsymbol{\beta}, \boldsymbol{\theta}) = \prod_{m=1}^M \int_0^\infty \mathcal{N}_1([D^T(\mathbf{y} - \boldsymbol{\mu})]_m; w_m A_m [D^T\boldsymbol{\beta}]_m, w_m A_m) \times f_{W_m}(w_m) dw_m \quad (10)$$

where $[D^T(\mathbf{y} - \boldsymbol{\mu})]_m$ denotes the m th component of vector $D^T(\mathbf{y} - \boldsymbol{\mu})$ and A_m the m th diagonal element of the diagonal matrix \boldsymbol{A} (or equivalently the m th eigenvalue of $\boldsymbol{\Sigma}$).

If we set $f_{W_m}(w_m)$ to a GIG distribution $\mathcal{GIG}(w_m; \lambda_m, \gamma_m, \delta_m)$, it follows that our generalization (MSGH) of the multivariate GH distribution with $\boldsymbol{\lambda} = [\lambda_1, \dots, \lambda_M]^T$, $\boldsymbol{\gamma} = [\gamma_1, \dots, \gamma_M]^T$ and $\boldsymbol{\delta} = [\delta_1, \dots, \delta_M]^T$ as M -dimensional vec-

tors is:

$$\begin{aligned} & \mathcal{MSGH}(\mathbf{y}; \boldsymbol{\mu}, \mathbf{D}, \mathbf{A}, \boldsymbol{\beta}, \boldsymbol{\lambda}, \boldsymbol{\gamma}, \boldsymbol{\delta}) \\ &= (2\pi)^{-M/2} \prod_{m=1}^M |A_m|^{-1/2} \left(\frac{\gamma_m}{\delta_m} \right)^{\lambda_m} \left(\frac{q_m(\mathbf{y})}{\alpha_m} \right)^{\lambda_m - 1/2} \times \\ & \quad K_{\lambda_m - 1/2}(q_m(\mathbf{y})\alpha_m) (K_{\lambda_m}(\delta_m\gamma_m))^{-1} \exp([\mathbf{D}^T(\mathbf{y} - \boldsymbol{\mu})]_m [\mathbf{D}^T\boldsymbol{\beta}]_m) \end{aligned} \quad (11)$$

with $\alpha_m^2 = \gamma_m^2 + A_m[\mathbf{D}^T\boldsymbol{\beta}]_m^2$ and $q_m(\mathbf{y})^2 = \delta_m^2 + A_m^{-1}[\mathbf{D}^T(\mathbf{y} - \boldsymbol{\mu})]_m^2$.
Alternatively, with $\mathbf{w} = [w_1, \dots, w_M]^T$ we can define it as

$$\begin{aligned} \mathbf{Y} | \mathbf{W} = \mathbf{w} & \sim \mathcal{N}_M(\boldsymbol{\mu} + \mathbf{D}\boldsymbol{\Delta}_{\mathbf{w}}\mathbf{A}\mathbf{D}^T\boldsymbol{\beta}, \mathbf{D}\boldsymbol{\Delta}_{\mathbf{w}}\mathbf{A}\mathbf{D}^T) \\ \mathbf{W} & \sim \mathcal{IG}(\lambda_1, \gamma_1, \delta_1) \otimes \dots \otimes \mathcal{IG}(\lambda_M, \gamma_M, \delta_M), \end{aligned} \quad (12)$$

where notation \otimes means that the \mathbf{W} components are independent. If we set $f_{W_m}(w_m)$ to an Inverse Gaussian distribution $\mathcal{IG}(w_m; \gamma_m, \delta_m)$, it follows that our generalization (MSNIG) of the multivariate NIG distribution with $\boldsymbol{\gamma}$ and $\boldsymbol{\delta}$ as M -dimensional vectors is:

$$\begin{aligned} \mathcal{MSNIG}(\mathbf{y}; \boldsymbol{\mu}, \mathbf{D}, \mathbf{A}, \boldsymbol{\beta}, \boldsymbol{\gamma}, \boldsymbol{\delta}) &= \prod_{m=1}^M \delta_m \exp(\delta_m\gamma_m + [\mathbf{D}^T(\mathbf{y} - \boldsymbol{\mu})]_m [\mathbf{D}^T\boldsymbol{\beta}]_m) \\ & \quad \times \frac{\alpha_m}{\pi q_m} K_1(\alpha_m q_m(\mathbf{y})) \end{aligned} \quad (13)$$

with $\alpha_m^2 = \gamma_m^2 + A_m[\mathbf{D}^T\boldsymbol{\beta}]_m^2$, $q_m(\mathbf{y})^2 = \delta_m^2 + A_m^{-1}[\mathbf{D}^T(\mathbf{y} - \boldsymbol{\mu})]_m^2$ and K_1 is the modified Bessel function of order 1.

To simulate from the MSGH distribution, it is possible to use (12) or

$$\mathbf{Y} = \boldsymbol{\mu} + \mathbf{D}\boldsymbol{\Delta}_{\mathbf{w}}\mathbf{A}\mathbf{D}^T\boldsymbol{\beta} + \mathbf{D}\mathbf{A}^{1/2}[X_1\sqrt{W_1}, \dots, X_M\sqrt{W_M}]^T \quad (14)$$

where $\mathbf{X} \sim \mathcal{N}(0, \mathbf{I}_M)$ and $W_m \sim \mathcal{IG}(\lambda_m, \gamma_m, \delta_m)$ (for $m = 1, \dots, M$).

It is interesting to note that the multiple scaled GH distribution allows potentially each dimension to follow a particular case of the GH distribution family. For example, in a bivariate setting $\mathbf{Y} = [Y_1, Y_2]^T$, the variate Y_1 could follow a hyperboloid distribution ($\lambda_1=0$) and Y_2 a NIG distribution ($\lambda_2 = -1/2$). In the case of assuming λ_m to be fixed, model choice criteria such as the Bayesian Information Criterion (BIC) could be used to discriminate between different model families.

2.3 Identifiability issues

In contrast to the standard multivariate GH distribution, constraining the determinant of \mathbf{A} to be 1 is not enough to ensure identifiability in the MSGH case. Indeed, assuming the determinant $|\mathbf{A}| = 1$, if we set $\mathbf{A}', \boldsymbol{\delta}', \boldsymbol{\gamma}'$ so that $A'_m = k_m^2 A_m$, $\delta'_m = \delta_m/k_m$ and $\gamma'_m = k_m\gamma_m$, for all values $k_1 \dots k_M$ satisfying $\prod_{m=1}^M k_m^2 = 1$, it follows that the determinant $|\mathbf{A}'| = 1$ and that the $\mathcal{MSGH}(\mathbf{y}; \boldsymbol{\mu}, \mathbf{D}, \mathbf{A}', \boldsymbol{\beta}, \boldsymbol{\lambda}, \boldsymbol{\gamma}', \boldsymbol{\delta}')$ and $\mathcal{MSGH}(\mathbf{y}; \boldsymbol{\mu}, \mathbf{D}, \mathbf{A}, \boldsymbol{\beta}, \boldsymbol{\lambda}, \boldsymbol{\gamma}, \boldsymbol{\delta})$ expressions are equal. Identifiability can be guaranteed by adding that all δ_m 's (or equivalently all γ_m 's) are equal. In practice, we will therefore assume that for all $m = 1 \dots M$, $\delta_m = \delta$.

2.4 Some properties of the multiple scaled GH distributions

The MSGH distribution (as defined in (11)) provides for very flexible distributional forms. For illustration, in the bivariate case, several contour plots of the multiple scaled NIG (*i.e.* for all m , $\lambda_m = -1/2$) are shown in Figure 1 and compared with the standard multivariate NIG. In this two-dimensional setting, we use for \mathbf{D} a parameterisation via an angle ξ so that $D_{11} = D_{22} = \cos \xi$ and $D_{21} = -D_{12} = \sin \xi$, where D_{md} denotes the (m, d) entry of matrix \mathbf{D} . Similar to the standard NIG the parameter β measures asymmetry and its sign determines the type of skewness. For the standard NIG the contours are not necessarily elliptical and this is also the case with the multiple scaled NIG. In the case of the multiple scaled NIG additional flexibility is provided by allowing the parameter γ to be a vector of dimension M instead of a scalar. Keeping all δ_m 's equal to the same δ , this vectorisation of γ effectively allows each dimension to be governed by different tail behaviour depending on the values of γ (see below).

Other multiple scaled and standard GH distributions are then also illustrated in Figure 1. As shown in Figure 1(g) and (i), changing λ_m values does not change much the shape of the contours but larger values of λ_m tend to produce heavier tails.

2.4.1 Mean and covariance matrix

Using the moments of the GIG distribution (see Jorgensen, 1982), *i.e.*, if W follows a $\mathcal{GIG}(\lambda, \gamma, \delta)$ distribution, for all $r \in \mathbb{Z}_+$,

$$E[W^r] = \left(\frac{\delta}{\gamma}\right)^r \frac{K_{\lambda+r}(\delta\gamma)}{K_{\lambda}(\delta\gamma)}, \quad (15)$$

it follows from representation (12) that when \mathbf{Y} follows a multiple scaled GH distribution,

$$\begin{aligned} E[\mathbf{Y}] &= E[E[\mathbf{Y}|\mathbf{W}]] = \boldsymbol{\mu} + \mathbf{D}E[\Delta_{\mathbf{w}}]\mathbf{A}\mathbf{D}^T\boldsymbol{\beta} \\ &= \boldsymbol{\mu} + \mathbf{D} \operatorname{diag}\left(\frac{\delta_m}{\gamma_m} \frac{K_{\lambda_m+1}(\delta_m\gamma_m)}{K_{\lambda_m}(\delta_m\gamma_m)}\right) \mathbf{A}\mathbf{D}^T\boldsymbol{\beta}, \end{aligned} \quad (16)$$

where for short, we denoted by $\operatorname{diag}(u_m)$ the M -dimensional diagonal matrix whose diagonal components are $\{u_1, \dots, u_M\}$.

For the covariance matrix, we get,

$$\operatorname{Var}[\mathbf{Y}] = E[\operatorname{Var}[\mathbf{Y}|\mathbf{W}]] + \operatorname{Var}[E[\mathbf{Y}|\mathbf{W}]] \quad (17)$$

$$\begin{aligned} &= \mathbf{D}E[\Delta_{\mathbf{w}}]\mathbf{A}\mathbf{D}^T + \mathbf{D}\mathbf{A} \operatorname{Var}[\Delta_{\mathbf{w}}\mathbf{D}^T\boldsymbol{\beta}]\mathbf{A}\mathbf{D}^T \\ &= \mathbf{D} \operatorname{diag}\left(\frac{\delta_m A_m}{\gamma_m} \frac{K_{\lambda_m+1}(\delta_m\gamma_m)}{K_{\lambda_m}(\delta_m\gamma_m)} \left(1 + \frac{\delta_m}{\gamma_m} [\mathbf{D}^T\boldsymbol{\beta}]_m^2 A_m\right.\right. \\ &\quad \left.\left. \times \left(\frac{K_{\lambda_m+2}(\delta_m\gamma_m)}{K_{\lambda_m+1}(\delta_m\gamma_m)} - \frac{K_{\lambda_m+1}(\delta_m\gamma_m)}{K_{\lambda_m}(\delta_m\gamma_m)}\right)\right)\right) \mathbf{D}^T \end{aligned} \quad (18)$$

For details of the mean and variance for the multiple scaled NIG distribution see Appendix A.

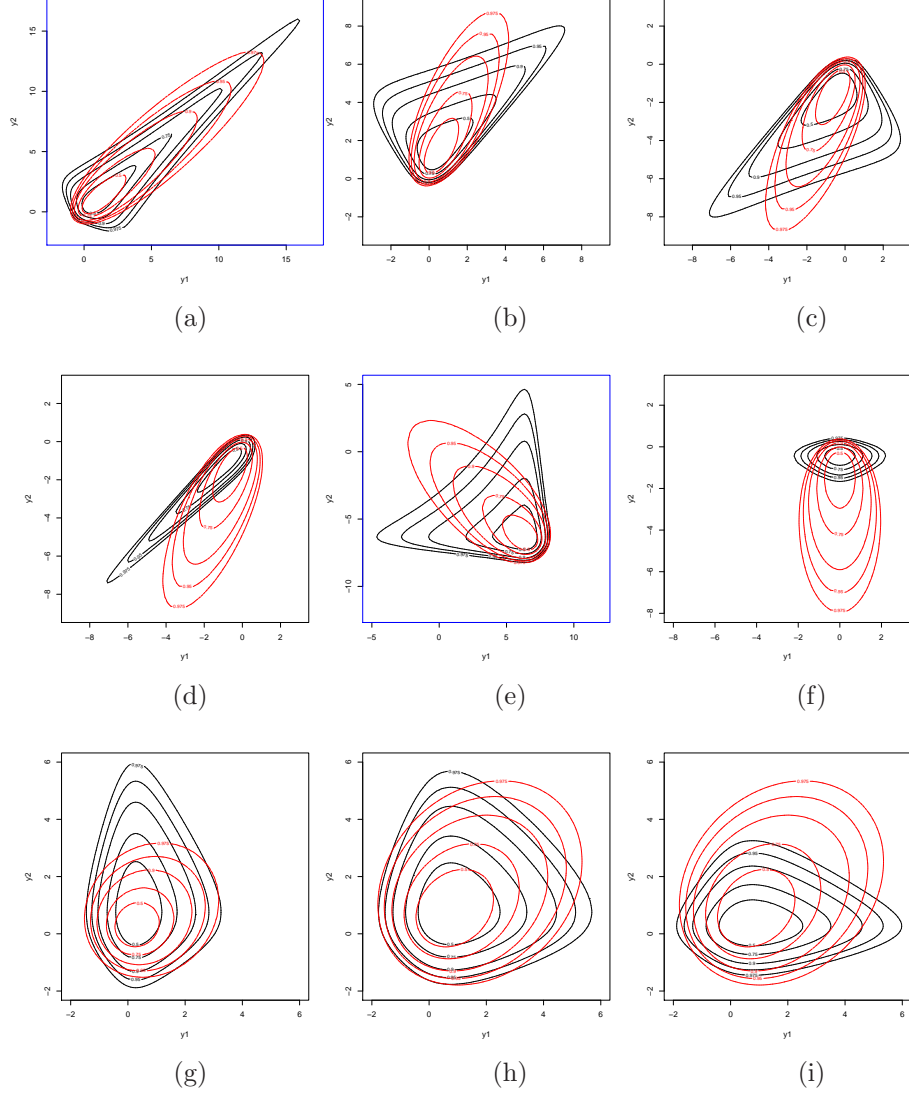


Figure 1: Top and middle panels: contour plots of bivariate multiple scaled NIG ($\lambda_1 = \lambda_2 = -1/2$) distributions (solid lines) with $\boldsymbol{\mu} = [0, 0]^T$ and $\boldsymbol{\delta} = \{1, 1\}$. The difference with the standard multivariate NIG (red dashed lines) is illustrated with univariate δ and γ values taken as the first respective component of the bivariate $\boldsymbol{\delta}$ and $\boldsymbol{\gamma}$. The (a-d) panels correspond to the same $\boldsymbol{\Sigma}$ built from $\mathbf{A} = \text{diag}(3/2, 2/3)$ and $\xi = \pi/4$ with (a) $\boldsymbol{\beta} = [2, 2]^T, \boldsymbol{\gamma} = [1, 1]^T$, (b) $\boldsymbol{\beta} = [0, 5]^T, \boldsymbol{\gamma} = [2, 2]^T$, (c) $\boldsymbol{\beta} = [0, -5]^T, \boldsymbol{\gamma} = [2, 2]^T$ and (d) $\boldsymbol{\beta} = [0, -5]^T, \boldsymbol{\gamma} = [2, 10]^T$. The (e,f) panels correspond to $\boldsymbol{\Sigma} = \mathbf{I}_2$ with (e) $\boldsymbol{\beta} = [-2, 2]^T, \boldsymbol{\gamma} = [1, 1]^T$, (f) $\boldsymbol{\beta} = [0, -5]^T, \boldsymbol{\gamma} = [1, 1]^T$. Bottom panels: contour plots of various multiple scaled (solid lines) and standard (red dashed lines) GH distributions all with $\boldsymbol{\Sigma} = \mathbf{I}_2, \boldsymbol{\beta} = [1, 1]^T, \boldsymbol{\gamma} = [2, 2]^T, \boldsymbol{\delta} = [1, 1]^T$ and (g) $\boldsymbol{\lambda} = [-1/2, 2]^T$, (h) $\boldsymbol{\lambda} = [-2, 2]^T$, (i) $\boldsymbol{\lambda} = [2, -1/2]^T$.

As can be seen from (17), the variance of the multiple scaled GH takes a slightly complicated form with some dependency on the skewness parameter β . This dependency is also present in the variance, recalled below, of the standard multivariate GH as given in (3),

$$\text{Var}[\mathbf{Y}_{GH}] = \frac{\delta}{\gamma} \frac{K_{\lambda+1}(\delta\gamma)}{K_{\lambda}(\delta\gamma)} \Sigma + \frac{\delta^2}{\gamma^2} \left(\frac{K_{\lambda+2}(\delta\gamma)}{K_{\lambda}(\delta\gamma)} - \frac{K_{\lambda+1}^2(\delta\gamma)}{K_{\lambda}^2(\delta\gamma)} \right) \Sigma \beta^T \beta \Sigma.$$

As noted recently by Arellano-Valle et al. (2007) and Lee and McLachlan (2012) an alternative form to allow separation between the skewness and the variance is provided in the case of the skew t distribution as parameterised by Sahu et al. (2003). Interestingly, other parameterisations of the skew- t distribution (Azzalini and Dalla Valle, 1996) do not share this separation property.

A notable difference between the covariance structure of the multiple scaled GH and the standard GH is that in the case of a diagonal scale matrix Σ , variates of the multiple scaled GH are independent of each other. Interestingly, this is not the case for the standard multivariate GH where the same latent factor W is shared across dimensions, and this effectively acts to induce some degree of dependency between dimensions (although they may be uncorrelated). A similar situation arises in the case of other distributions with shared latent factors, for example the standard t -distribution. As mentioned previously, in the multiple scaled GH case the latent factor W is allowed to vary independently across dimensions.

The tail behaviour of the multiple scaled GH is similar to the GH with tails governed by a combined algebraic and exponential form equivalent to $\delta \exp(\delta\gamma_m + [\mathbf{D}^T \mathbf{y}]_{(m)} [\mathbf{D}^T \beta]_{(m)} - \alpha_m q_m(\mathbf{y})) q_m(\mathbf{y})^{-1}$, where q_m and α_m are defined in Equation (11). Hence, the multiple scaled GH, like the GH distribution, is said to be *semi-heavy* tailed, which means that its tail behaviour is characterized by exponential instead of power decay. Alternative parameterisations of the GH permit the possibility of heavier tails (Aas and Hobaek Haff, 2006). The parameters γ , δ and β govern the tail behaviour of the density with smaller values of γ and δ implying heavier tails, and larger values lighter tails. For our multiple scaled GH distributions, when all δ_m, γ_m tend to infinity with δ_m/γ_m tending to 1, the distribution tends to the multivariate Gaussian $\mathcal{N}(\mu + \Sigma\beta, \Sigma)$. This is easily seen from the characteristic function (see Section 2.4.2).

A difference between the tail behaviour of the GH and the multiple scaled GH can also be seen in measures of the tail dependency (Coles et al., 1999). In applications, strong tail dependence is important for modelling the dependency/association of potentially extreme events (*e.g.* in finance, meteorology). In Figure 2 we compare the tail dependency of the Gaussian, t -distribution, standard GH and multiple scaled GH using a $\chi(q)$ plot (Coles et al., 1999) and simulated values from each distribution with $\mu = [0, 0]^T$, $\Sigma = \begin{pmatrix} 1 & 0.5 \\ 0.5 & 1 \end{pmatrix}$ (equivalently $\mathbf{A} = \text{diag}(3/2, 1/2)$ and $\xi = \pi/4$), $\beta = [0, 0]^T$, $\gamma = \delta = [1, 1]^T$ (or $\nu = 1$) and $\lambda = [-1/2, -1/2]^T$ (NIG). The function $\chi(q)$ can be interpreted as a quantile dependent measure of dependence with $\chi(q) = 0$ indicating independence and $\chi(q) = 1$ perfect dependence (For further details see Appendix D). Tail dependence is determined by the limit of $\chi(q)$ when q tends to 1.

From Figure 2, we see that the multiple scaled NIG has stronger tail dependence than the standard NIG. By comparison (and for reference), it is

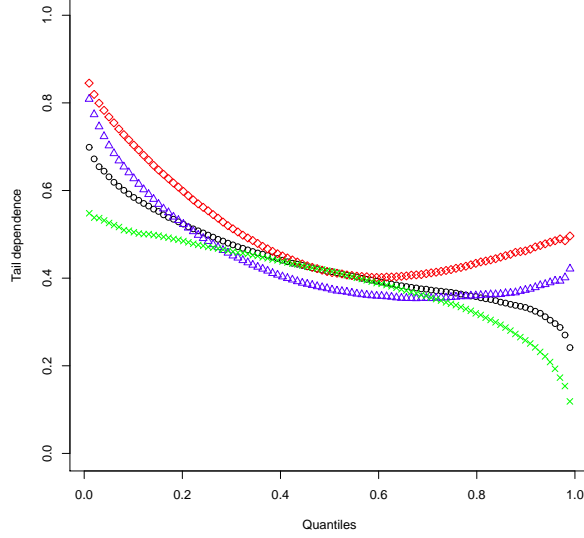


Figure 2: Comparison of tail dependence using $\chi(q)$. X-axis: quantiles levels. Y-axis: Estimate of $\chi(q)$, dashed lines indicate the 95% confidence interval. Gaussian distribution (Green), Standard NIG distribution (black), Multiple scaled NIG distribution (blue), t distribution (Red)

well known that the Gaussian distribution has no tail dependence, and the t -distribution has a stronger tail dependence than both the Gaussian and the standard NIG.

2.4.2 Characteristic function

Denote by $\phi_{\mathbf{Y}}$ the characteristic function of a random vector \mathbf{Y} . It follows from (14) that, $\forall \mathbf{t} \in \mathbb{R}^M$, $\phi_{\mathbf{Y}}(\mathbf{t}) = E[\exp(it^T \mathbf{Y})] = E[E[\exp(it^T \mathbf{Y})|W]] = \exp(it^T \boldsymbol{\mu}) \prod_{m=1}^M \phi_{W_m}(u_m(\mathbf{t}))$.

where $u_m(\mathbf{t}) = [A^{1/2} D^T \mathbf{t}]_m ([A^{1/2} D^T \boldsymbol{\beta}]_m + \frac{i}{2} [A^{1/2} D^T \mathbf{t}]_m)$ and ϕ_{W_m} is the characteristic function of W_m .

In the Generalised Hyperbolic case ϕ_{W_m} is the characteristic function of a 1-dimensional $\mathcal{GIG}(\lambda_m, \gamma_m, \delta_m)$ distribution, which is

$$\phi_{W_m}(t) = \left(\frac{\gamma_m}{\gamma_m - 2it} \right)^{\lambda_m} \frac{K_{\lambda_m}(\delta_m \sqrt{\gamma_m^2 - 2it})}{K_{\lambda_m}(\delta_m \gamma_m)}. \quad (19)$$

The particular case of the multiple scaled NIG follows easily by setting $\lambda_m = -1/2$, which permits a simpler form

$$\phi_{W_m}(t) = \exp(\delta_m \gamma_m - \delta_m \sqrt{\gamma_m^2 - 2it}). \quad (20)$$

The characteristic function is useful in practice for the computation of marginals as detailed in the next section.

2.4.3 Marginals

Using (12), marginals are easy to sample from but computing their pdfs involves, in general, numerical integration. An efficient and simple algorithm to compute such marginal pdfs in most cases can be derived according to Shephard (1991). The derivation in Shephard (1991) is based on the inversion formula of the characteristic function which in the univariate case is:

$$\begin{aligned} f_Y(y) &= \frac{1}{2\pi} \int_0^\infty (\exp(iy)\phi_Y(-t) + \exp(-iy)\phi_Y(t))dt \\ &= \frac{1}{\pi} \int_0^\infty \text{Re}(\exp(-iy)\phi_Y(t))dt \end{aligned} \quad (21)$$

using the hermitian property of characteristic functions $\phi_Y(-t) = \overline{\phi_Y(t)}$ (the over line means the complex conjugate).

As an illustration, Figure 3 shows plots of the pdf of some 1-D marginals and a comparison with 1-D NIG distributions. From Figure 3 we can see that the marginals of the proposed multiple scaled NIG (MSNIG) distribution deviate slightly from the standard NIG distribution according to the specification of Σ . The marginals of the MSNIG distribution are exactly 1-D standard NIG distributions in the diagonal scale matrix case.

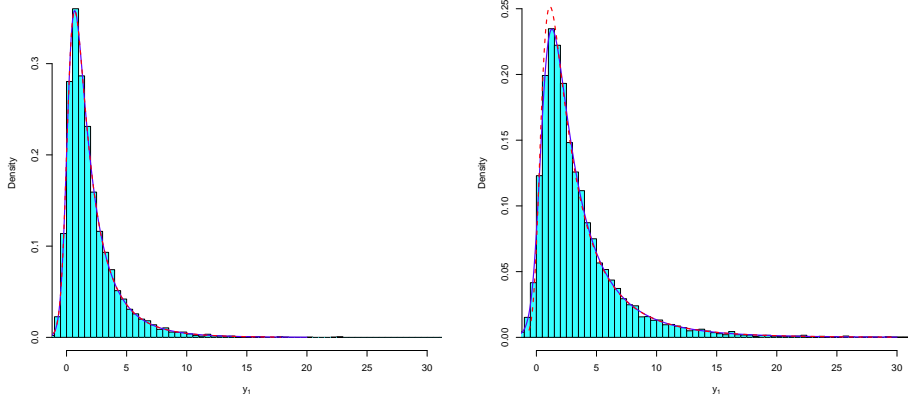


Figure 3: Histogram and density plots of the marginal \mathbf{Y}_1 of a bivariate NIG distribution with $\boldsymbol{\mu} = [0, 0]^T$, $\boldsymbol{\gamma} = \boldsymbol{\delta} = \boldsymbol{\beta} = [2, 2]^T$, and (left) diagonal Σ with diagonal entries equal to 1 or (right) Σ with diagonal entries equal to 1 and other entries to 0.5. Histograms and blue solid lines denote the multiple scaled NIG and red dashed lines the standard NIG.

For marginals of dimension greater than 1, we can also easily derive the characteristic function and use a simple multidimensional inversion formula. Let \mathcal{I} be a subset of $\{1, \dots, M\}$ of size I and write $\mathbf{Y}_{\mathcal{I}} = \{Y_m, m \in \mathcal{I}\}$ and $\mathbf{t}_{\mathcal{I}} = \{t_m, m \in \mathcal{I}\}$. The characteristic function of the marginal variable $\mathbf{Y}_{\mathcal{I}}$ is

$$\phi_{\mathbf{Y}_{\mathcal{I}}}(\mathbf{t}_{\mathcal{I}}) = \prod_{m \in \mathcal{I}} \exp(it_m \mu_m) \prod_{d=1}^M \phi_{W_d}(u_d(\mathbf{t}_{\mathcal{I}})), \quad (22)$$

with $u_d(\mathbf{t}_{\mathcal{I}}) = (\sum_{m \in \mathcal{I}} t_m [\mathbf{D} \mathbf{A}^{1/2}]_{md} [\mathbf{A}^{1/2} \mathbf{D}^T \boldsymbol{\beta}]_d) + \frac{i}{2} (\sum_{m \in \mathcal{I}} t_m [\mathbf{D} \mathbf{A}^{1/2}]_{md})^2$.

It follows that the density of $\mathbf{Y}_{\mathcal{I}}$ via the multidimensional inversion formula (see *e.g.* Shephard (1991)) is:

$$f_{\mathbf{Y}_{\mathcal{I}}}(\mathbf{y}_{\mathcal{I}}) = (2\pi)^{-I} \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} \exp(-i \mathbf{t}_{\mathcal{I}}^T \mathbf{y}_{\mathcal{I}}) \phi_{\mathbf{Y}_{\mathcal{I}}}(\mathbf{t}_{\mathcal{I}}) d\mathbf{t}_{\mathcal{I}} \quad (23)$$

When $I = 2$, and decomposing \mathbb{R}^2 into four quadrants,

$$f_{\mathbf{Y}_{\mathcal{I}}}(\mathbf{y}_{\mathcal{I}}) = 2 (2\pi)^{-2} \int_0^{\infty} \int_{-\infty}^{\infty} \text{Re}(\exp(-i \mathbf{t}_{\mathcal{I}}^T \mathbf{y}_{\mathcal{I}}) \phi_{\mathbf{Y}_{\mathcal{I}}}(\mathbf{t}_{\mathcal{I}})) d\mathbf{t}_{\mathcal{I}}. \quad (24)$$

This formula also generalizes easily in higher dimensions.

For illustration, Figure 4 shows the bivariate marginal $[Y_1, Y_2]^T$ for a 3 dimensional $[Y_1, Y_2, Y_3]^T$ following a MSNIG distribution with $\boldsymbol{\mu} = [0, 0, 0]^T$, $\boldsymbol{\gamma} = \boldsymbol{\delta} = [3, 3, 3]^T$, $\boldsymbol{\beta} = [-6, 2, 2]^T$ and $\boldsymbol{\Sigma}$ so that its diagonal entries are 1 and other entries are 0.5. It is clear from the shape of the contours that this bivariate marginal takes a slightly different shape to a bivariate standard NIG distribution.

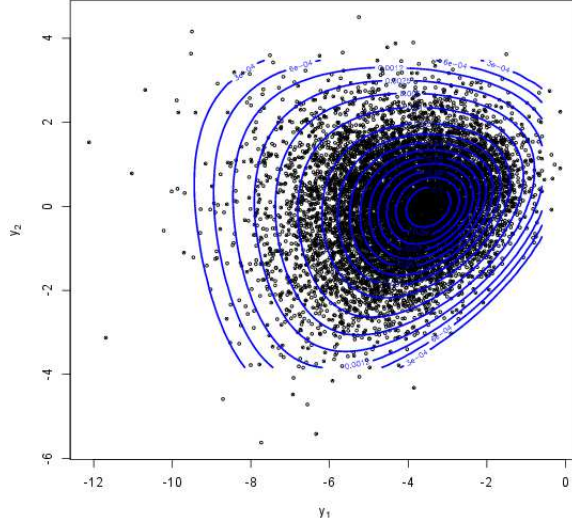


Figure 4: $[Y_1, Y_2]^T$ distribution when $[Y_1, Y_2, Y_3]^T$ follows a multiple scaled trivariate NIG distribution with $\boldsymbol{\mu} = [0, 0, 0]^T$, $\boldsymbol{\gamma} = \boldsymbol{\delta} = [3, 3, 3]^T$, $\boldsymbol{\beta} = [-6, 2, 2]^T$ and $\boldsymbol{\Sigma}$ so that its diagonal entries are 1 and other entries are 0.5. Contours are superimposed on points sampled from the distribution using equation (12).

3 Maximum likelihood estimation of parameters

In this section, for illustration we outline an EM approach to estimate the parameters of the multiple scaled NIG distribution as it appears to be the most

popular case of the GH family used in applications especially in finance. As noted also by (Protassov, 2004; Barndorff-Nielsen, 1997), for the GH distribution it can be very difficult to show a significant difference between different values of λ due to the flatness of the likelihood and computational difficulties arise in some cases where the likelihood can be infinite. For these reasons we outline the particular case of allowing all λ_m 's to be fixed but we note that it is relatively straightforward to extend our proposed approach to the more general case. Also for identifiability reasons, we set all δ_m 's to the same δ value so that the parameters to estimate in the multiple scaled NIG case are $\Psi = \{\boldsymbol{\mu}, \mathbf{D}, \mathbf{A}, \boldsymbol{\beta}, \boldsymbol{\gamma}, \delta\}$ with $|\mathbf{A}| = 1$.

Estimation of most of the parameters for the multiple scaled NIG distribution is relatively straightforward but the separate estimation of \mathbf{D} and \mathbf{A} requires an additional minimization algorithm based on the Flury and Gautschi algorithm (Flury, 1984; Flury and Gautschi, 1986). Similar difficulties are also encountered in Gaussian model-based clustering (Celeux and Govaert, 1995) for some of the proposed models.

Let us consider an *i.i.d* sample $\mathbf{y} = \{\mathbf{y}_1, \dots, \mathbf{y}_N\}$ of the multiple scaled NIG distribution defined in (13). As in the standard NIG distribution case (Karlis, 2002), a convenient computational advantage of the EM approach is to view the weights as an additional missing variable \mathbf{W} . The observed data \mathbf{y} are seen as being incomplete and additional missing weight variables $\mathbf{W}_1 \dots \mathbf{W}_N$ with for $i \in \{1 \dots N\}$, $\mathbf{W}_i = [W_{i1} \dots W_{iM}]^T$ are introduced. These weights are defined so that $\forall i \in \{1 \dots N\}$:

$$\begin{aligned} \mathbf{Y}_i | \mathbf{W}_i = \mathbf{w}_i &\sim \mathcal{N}_M(\boldsymbol{\mu} + \mathbf{D}\boldsymbol{\Delta}_{\mathbf{w}_i}\mathbf{A}\mathbf{D}^T\boldsymbol{\beta}, \mathbf{D}\boldsymbol{\Delta}_{\mathbf{w}_i}\mathbf{A}\mathbf{D}^T) \\ \text{and } \mathbf{W}_i &\sim \mathcal{IG}(\gamma_1, \delta) \otimes \dots \otimes \mathcal{IG}(\gamma_M, \delta) \end{aligned} \quad (25)$$

where $\boldsymbol{\Delta}_{\mathbf{w}_i} = \text{diag}(w_{i1}, \dots, w_{iM})$.

As a way of circumventing the restriction that the determinant $|\mathbf{A}| = 1$ in the M-step, representation (25) above can be rewritten equivalently as,

$$\begin{aligned} \mathbf{Y}_i | \mathbf{W}_i = \mathbf{w}_i &\sim \mathcal{N}_M(\boldsymbol{\mu} + \mathbf{D}\boldsymbol{\Delta}_{\mathbf{w}_i}\mathbf{D}^T\tilde{\boldsymbol{\beta}}, \mathbf{D}\boldsymbol{\Delta}_{\mathbf{w}_i}\tilde{\mathbf{A}}\mathbf{D}^T) \\ \mathbf{W}_i &\sim \mathcal{IG}(\tilde{\gamma}_1, 1) \otimes \dots \otimes \mathcal{IG}(\tilde{\gamma}_M, 1) \end{aligned} \quad (26)$$

where

$$\begin{aligned} \tilde{\mathbf{A}} &= \delta^2 \mathbf{A} \\ \tilde{\boldsymbol{\beta}} &= \mathbf{D}\tilde{\mathbf{A}}\mathbf{D}^T\boldsymbol{\beta} \\ \tilde{\boldsymbol{\gamma}} &= \delta \boldsymbol{\gamma} \end{aligned}$$

and $\tilde{\mathbf{A}}$ is now a general (positive definite) diagonal matrix. Note that in the location term in the definition above (26), $\mathbf{D}\boldsymbol{\Delta}_{\mathbf{w}_i}\mathbf{D}^T\tilde{\boldsymbol{\beta}} = \mathbf{D}\boldsymbol{\Delta}_{\mathbf{w}_i}\tilde{\mathbf{A}}\mathbf{D}^T\boldsymbol{\beta}$.

3.1 E step

At iteration (r) with $\boldsymbol{\psi}^{(r)}$ being the current parameter value, the E-step leads to the computation for all $i = 1, \dots, N$, of the missing variables posterior distributions $p(\mathbf{w}_i | \mathbf{y}_i; \boldsymbol{\psi}^{(r)})$. It consists then of calculating $p(\mathbf{w}_i | \mathbf{y}_i; \boldsymbol{\psi}^{(r)}) \propto p(\mathbf{y}_i | \mathbf{w}_i; \boldsymbol{\psi}^{(r)})p(\mathbf{w}_i; \boldsymbol{\psi}^{(r)})$ which can be shown (see Appendix of Karlis and Santourian,

2009) to follow a Generalised Inverse Gaussian distribution (see definition (2)). In our case, and assuming the \mathbf{W}_i 's are independent we have,

$$p(\mathbf{w}_i|\mathbf{y}_i; \boldsymbol{\psi}^{(r)}) = \prod_{m=1}^M \mathcal{GIG}(w_{im}; -1, \hat{\alpha}_m^{(r)}, \phi_{im}^{(r)}), \quad (27)$$

where

$$\begin{aligned} \phi_{im}^{(r)} &= \sqrt{1 + \frac{[\mathbf{D}^{(r)T}(\mathbf{y}_i - \boldsymbol{\mu}^{(r)})]_m^2}{\tilde{\mathbf{A}}_m^{(r)}}} \\ \hat{\alpha}_m^{(r)} &= \sqrt{\tilde{\gamma}_m^{(r)2} + \frac{[\mathbf{D}^{(r)T}\tilde{\boldsymbol{\beta}}^{(r)}]_m^2}{\tilde{\mathbf{A}}_m^{(r)}}}. \end{aligned}$$

As all moments of a Generalised Inverse Gaussian distribution exist (see (15)), it follows that we have closed form expressions for the following quantities needed in the E-step,

$$\begin{aligned} s_{im}^{(r)} &= E[W_{im}|\mathbf{y}_i; \boldsymbol{\psi}^{(r)}] = \frac{\phi_{im}^{(r)} K_0(\phi_{im}^{(r)} \hat{\alpha}_m^{(r)})}{\hat{\alpha}_m^{(r)} K_{-1}(\phi_{im}^{(r)} \hat{\alpha}_m^{(r)})} \\ t_{im}^{(r)} &= E[W_{im}^{-1}|\mathbf{y}_i; \boldsymbol{\psi}^{(r)}] = \frac{\hat{\alpha}_m^{(r)} K_{-2}(\phi_{im}^{(r)} \hat{\alpha}_m^{(r)})}{\phi_{im}^{(r)} K_{-1}(\phi_{im}^{(r)} \hat{\alpha}_m^{(r)})}. \end{aligned}$$

Note that equivalently $K_{-1} = K_1$ and $K_{-2} = K_2$. The Bessel function can be numerically evaluated in most statistical packages. All computations in this paper were undertaken using R (Team, 2011).

3.2 M step

For the updating of $\boldsymbol{\psi}$, the M-step consists of two independent steps for $(\boldsymbol{\mu}, \mathbf{D}, \tilde{\mathbf{A}}, \tilde{\boldsymbol{\beta}})$ and $\tilde{\gamma}$,

$$\begin{aligned} (\boldsymbol{\mu}, \mathbf{D}, \tilde{\mathbf{A}}, \tilde{\boldsymbol{\beta}})^{(r+1)} &= \arg \max_{\boldsymbol{\mu}, \mathbf{D}, \tilde{\mathbf{A}}, \tilde{\boldsymbol{\beta}}} \sum_{i=1}^N E[\log p(\mathbf{y}_i, |\mathbf{W}_i; \boldsymbol{\mu}, \mathbf{D}, \tilde{\mathbf{A}}, \tilde{\boldsymbol{\beta}})|\mathbf{y}_i, \boldsymbol{\psi}^{(r)}] \quad (28) \\ &= \arg \max_{\boldsymbol{\mu}, \mathbf{D}, \tilde{\mathbf{A}}, \tilde{\boldsymbol{\beta}}} \left\{ \sum_{i=1}^N -\frac{1}{2} \log |\tilde{\mathbf{A}}| - \frac{1}{2} (\mathbf{y}_i - \boldsymbol{\mu} - \mathbf{D} \mathbf{S}_i^{(r)} \mathbf{D}^T \tilde{\boldsymbol{\beta}})^T \right. \\ &\quad \times \left. \mathbf{D} \tilde{\mathbf{A}}^{-1} \mathbf{T}_i^{(r)} \mathbf{D}^T (\mathbf{y}_i - \boldsymbol{\mu} - \mathbf{D} \mathbf{S}_i^{(r)} \mathbf{D}^T \tilde{\boldsymbol{\beta}}) \right\} \end{aligned}$$

and

$$\begin{aligned} \tilde{\gamma}^{(r+1)} &= \arg \max_{\tilde{\gamma}} \sum_{i=1}^N \sum_{m=1}^M E[\log p(W_{im}; \tilde{\gamma}_m, 1)|\mathbf{y}_i, \boldsymbol{\psi}^{(r)}] \quad (29) \\ &= \arg \max_{\tilde{\gamma}} \left\{ \sum_{i=1}^N \sum_{m=1}^M \tilde{\gamma}_m - \frac{1}{2} \tilde{\gamma}_m^2 s_{im}^{(r)} \right\} \end{aligned}$$

where $\mathbf{T}_i^{(r)} = \text{diag}(t_{i1}^{(r)}, \dots, t_{iM}^{(r)})$ and $\mathbf{S}_i^{(r)} = \text{diag}(s_{i1}^{(r)}, \dots, s_{iM}^{(r)})$ and ignoring constants.

The optimization of these steps leads to the following update equations.

Updating $\boldsymbol{\mu}$. It follows from (28) that for fixed \mathbf{D} and \mathbf{A} (ignoring constants)

$$\boldsymbol{\mu}^{(r+1)} = \arg \min_{\boldsymbol{\mu}} \left\{ \sum_{i=1}^N (\mathbf{y}_i - \boldsymbol{\mu} - \mathbf{D} \mathbf{S}_i^{(r)} \mathbf{D}^T \tilde{\boldsymbol{\beta}})^T \mathbf{D} \tilde{\mathbf{A}}^{-1} \mathbf{T}_i^{(r)} \mathbf{D}^T (\mathbf{y}_i - \boldsymbol{\mu} - \mathbf{D} \mathbf{S}_i^{(r)} \mathbf{D}^T \tilde{\boldsymbol{\beta}}) \right\} \quad (30)$$

which by fixing \mathbf{D} to the current estimation $\mathbf{D}^{(r)}$, leads to

$$\begin{aligned} \boldsymbol{\mu}^{(r+1)} = & \left(\frac{\sum_{i=1}^N \mathbf{T}_i^{(r)} \mathbf{D}^{(r)T}}{N} - N \left(\sum_{i=1}^N \mathbf{S}_i^{(r)} \right)^{-1} \right)^{-1} \\ & \times \left(\frac{\sum_{i=1}^N \mathbf{T}_i^{(r)} \mathbf{D}^{(r)T} \mathbf{y}_i}{N} - \sum_{i=1}^N \mathbf{y}_i \left(\sum_{i=1}^N \mathbf{S}_i^{(r)} \right)^{-1} \right) \end{aligned}$$

Updating $\tilde{\boldsymbol{\beta}}$. To update $\tilde{\boldsymbol{\beta}}$ we have to minimize the following quantity,

$$\tilde{\boldsymbol{\beta}}^{(r+1)} = \arg \min_{\tilde{\boldsymbol{\beta}}} \left\{ \sum_{i=1}^N (\mathbf{y}_i - \boldsymbol{\mu} - \mathbf{D} \mathbf{S}_i^{(r)} \mathbf{D}^T \tilde{\boldsymbol{\beta}})^T \mathbf{D} \tilde{\mathbf{A}}^{-1} \mathbf{T}_i^{(r)} \mathbf{D}^T (\mathbf{y}_i - \boldsymbol{\mu} - \mathbf{D} \mathbf{S}_i^{(r)} \mathbf{D}^T \tilde{\boldsymbol{\beta}}) \right\} \quad (31)$$

which by fixing \mathbf{D} and $\boldsymbol{\mu}$ to their current estimations $\mathbf{D}^{(r)}$ and $\boldsymbol{\mu}^{(r+1)}$, leads to

$$\tilde{\boldsymbol{\beta}}^{(r+1)} = \mathbf{D}^{(r)} \left(\sum_{i=1}^N \mathbf{S}_i^{(r)} \right)^{-1} \mathbf{D}^{(r)T} \sum_{i=1}^N (\mathbf{y}_i - \boldsymbol{\mu}^{(r+1)})$$

Updating \mathbf{D} . Using the equality $x^T \mathbf{S} x = \text{trace}(\mathbf{S} x x^T)$ for any matrix \mathbf{S} , it follows that for fixed $\tilde{\mathbf{A}}$ and $\boldsymbol{\mu}$, \mathbf{D} is obtained by minimizing

$$\begin{aligned} \mathbf{D}^{(r+1)} = \arg \min_{\mathbf{D}} \left\{ \sum_{i=1}^N \text{trace}(\mathbf{D} \mathbf{T}_i^{(r)} \tilde{\mathbf{A}}^{(r)-1} \mathbf{D}^T \mathbf{V}_i) + \sum_{i=1}^N \text{trace}(\mathbf{D} \mathbf{S}_i^{(r)} \tilde{\mathbf{A}}^{(r)-1} \mathbf{D}^T \mathbf{B}_i) \right. \\ \left. - 2 \sum_{i=1}^N \text{trace}(\mathbf{D} \tilde{\mathbf{A}}^{(r)-1} \mathbf{D}^T \mathbf{C}_i) \right\} \end{aligned}$$

where $\mathbf{V}_i = (\mathbf{y}_i - \boldsymbol{\mu}^{(r+1)})(\mathbf{y}_i - \boldsymbol{\mu}^{(r+1)})^T$, $\mathbf{B}_i = \tilde{\boldsymbol{\beta}}^{(r+1)} \tilde{\boldsymbol{\beta}}^{(r+1)T}$, $\mathbf{C}_i = (\mathbf{y}_i - \boldsymbol{\mu}^{(r+1)}) \tilde{\boldsymbol{\beta}}^{(r+1)T}$.

Using current values $\boldsymbol{\mu}^{(r+1)}$, $\tilde{\boldsymbol{\beta}}^{(r+1)}$ and $\tilde{\mathbf{A}}^{(r)}$, the parameter \mathbf{D} can be updated using an algorithm derived from Flury and Gautschi (see Celeux and Govaert (1995)) which is outlined in Appendix B.

Updating $\tilde{\mathbf{A}}$. To update $\tilde{\mathbf{A}}$ we have to minimize the following quantity

$$\begin{aligned}
\tilde{\mathbf{A}}^{(r+1)} &= \arg \min_{\tilde{\mathbf{A}}} \left\{ \sum_{i=1}^N \text{trace}(\mathbf{D}^{(r+1)} \mathbf{T}_i^{(r)} \tilde{\mathbf{A}}^{-1} \mathbf{D}^{(r+1)T} \mathbf{V}_i) \right. \\
&\quad + \sum_{i=1}^N \text{trace}(\mathbf{D}^{(r+1)} \mathbf{S}_i^{(r)} \tilde{\mathbf{A}}^{-1} \mathbf{D}^{(r+1)T} \mathbf{B}_i^{(r)}) - \\
&\quad \left. 2 \sum_{i=1}^N \text{trace}(\mathbf{D}^{(r+1)} \tilde{\mathbf{A}}^{-1} \mathbf{D}^{(r+1)T} \mathbf{C}_i) + N \log |\tilde{\mathbf{A}}| \right\} \\
&= \arg \min_{\tilde{\mathbf{A}}} \left\{ \text{trace} \left[\sum_{i=1}^N (\mathbf{T}_i^{(r)1/2} \mathbf{D}^{(r+1)T} \mathbf{V}_i \mathbf{D}^{(r+1)} \mathbf{T}_i^{(r)1/2} + \right. \right. \\
&\quad \left. \left. \mathbf{S}_i^{(r)1/2} \mathbf{D}^{(r+1)T} \mathbf{B}_i \mathbf{D}^{(r+1)} \mathbf{S}_i^{(r)1/2} - \mathbf{D}^{(r+1)T} (\mathbf{C}_i + \mathbf{C}_i^T) \mathbf{D}^{(r+1)}) \tilde{\mathbf{A}}^{-1} \right] \right. \\
&\quad \left. + N \log |\tilde{\mathbf{A}}| \right\} \\
&= \arg \min_{\tilde{\mathbf{A}}} \left\{ \text{trace} \left(\left(\sum_{i=1}^N \mathbf{M}_i \right) \tilde{\mathbf{A}}^{-1} \right) + N \log \tilde{\mathbf{A}} \right\}
\end{aligned}$$

where $\mathbf{M}_i = \mathbf{T}_i^{(r)1/2} \mathbf{D}^{(r+1)T} \mathbf{V}_i \mathbf{D}^{(r+1)} \mathbf{T}_i^{(r)1/2} + \mathbf{S}_i^{(r)1/2} \mathbf{D}^{(r+1)T} \mathbf{B}_i \mathbf{D}^{(r+1)} \mathbf{S}_i^{(r)1/2} - \mathbf{D}^{(r+1)T} (\mathbf{C}_i + \mathbf{C}_i^T) \mathbf{D}^{(r+1)}$ and \mathbf{M}_i is a symmetric positive definite matrix.

We can use the following corollary (see Corollary A-2 in Celeux and Govaert (1995)) with $\mathbf{S} = \sum_{i=1}^N \mathbf{M}_i$.

Corollary 3.2: *The $M \times M$ diagonal matrix \mathbf{A} minimizing $\text{trace}(\mathbf{S}\mathbf{A}^{-1}) + \alpha \log |\mathbf{A}|$ where \mathbf{S} is a $M \times M$ symmetric definite positive matrix and α is a positive real number is $\mathbf{A} = \frac{\text{diag}(\mathbf{S})}{\alpha}$*

By setting \mathbf{D} and $\boldsymbol{\mu}$ to their current estimations $\mathbf{D}^{(r+1)}$ and $\boldsymbol{\mu}^{(r+1)}$ we then get,

$$\tilde{\mathbf{A}}^{(r+1)} = \frac{\text{diag}(\mathbf{S})}{N} \quad (32)$$

where

$$\begin{aligned}
\mathbf{S} &= \sum_{i=1}^N (\mathbf{T}_i^{(r)1/2} \mathbf{D}^{(r+1)T} \mathbf{V}_i \mathbf{D}^{(r+1)} \mathbf{T}_i^{(r)1/2} + \mathbf{S}_i^{(r)1/2} \mathbf{D}^{(r+1)T} \mathbf{B}_i \mathbf{D}^{(r+1)} \mathbf{S}_i^{(r)1/2} \\
&\quad - \mathbf{D}^{(r+1)T} (\mathbf{C}_i + \mathbf{C}_i^T) \mathbf{D}^{(r+1)}) .
\end{aligned} \quad (33)$$

Equivalently, for all m

$$\begin{aligned}
\tilde{\mathbf{A}}_m^{(r+1)} &= \frac{1}{N} \sum_{i=1}^N \left([\mathbf{D}^{(r+1)T} (\mathbf{y}_i - \boldsymbol{\mu}^{(r+1)})]_m^2 t_{im}^{(r)} + [\mathbf{D}^{(r+1)T} \tilde{\boldsymbol{\beta}}^{(r+1)}]_m^2 s_{im}^{(r)} \right. \\
&\quad \left. - 2 [\mathbf{D}^{(r+1)T} (\mathbf{y}_i - \boldsymbol{\mu}^{(r+1)})]_m [\mathbf{D}^{(r+1)T} \tilde{\boldsymbol{\beta}}^{(r+1)}]_m \right)
\end{aligned} \quad (34)$$

Updating $\tilde{\gamma}$. It follows from (29) that to update $\tilde{\gamma}$ we have to minimize,

$$\tilde{\gamma}_m^{(r+1)} = \arg \min_{\tilde{\gamma}} \left\{ \sum_{i=1}^N \sum_{m=1}^M \frac{1}{2} \tilde{\gamma}_m^2 s_{im}^{(r)} - \tilde{\gamma}_m \right\} \quad (35)$$

which for all $m = 1, \dots, M$ leads to,

$$\tilde{\gamma}_m^{(r+1)} = \frac{N}{\sum_{i=1}^N s_{im}^{(r)}}.$$

Updating constrained $\tilde{\gamma}$. Similar updating equations can be easily derived when $\tilde{\gamma}$ is assumed to be equal for several dimensions. If we assume that for all m , $\tilde{\gamma}_m = \tilde{\gamma}$ then

$$\tilde{\gamma}^{(r+1)} = \frac{NM}{\sum_{i=1}^N \sum_{m=1}^M s_{im}^{(r)}}$$

It is also quite easy to extend the above equation to the case where $\tilde{\gamma}$ is assumed to be equal for only some of the dimensions. For either case, model choice criteria could be used to justify the appropriateness of the assumed parameter space for $\tilde{\gamma}$.

Eventually, to transform the estimated parameters back to their original form we can take $\delta = |\tilde{\mathbf{A}}|^{\frac{1}{2M}}$, $\gamma_m = \tilde{\gamma}_m / \delta$, $\beta = \mathbf{D} \tilde{\mathbf{A}}^{-1} \mathbf{D}^T \tilde{\beta}$ and $\mathbf{A} = \tilde{\mathbf{A}} / |\tilde{\mathbf{A}}|^{1/M}$.

3.3 Mixture of multiple scaled NIG distributions

The previous results can be extended to cover the case of K -component mixture of multiple scaled NIG distributions. With the usual notation for the proportions $\boldsymbol{\pi} = \{\pi_1, \dots, \pi_K\}$ and $\boldsymbol{\psi}_k = \{\boldsymbol{\mu}_k, \mathbf{D}_k, \mathbf{A}_k, \boldsymbol{\beta}_k, \gamma_k, \delta_k\}$ for $k = 1 \dots K$, we consider,

$$p(\mathbf{y}; \boldsymbol{\phi}) = \sum_{k=1}^K \pi_k \mathcal{MSNIG}(\mathbf{y}; \boldsymbol{\mu}_k, \mathbf{D}_k, \mathbf{A}_k, \boldsymbol{\beta}_k, \gamma_k, \delta_k)$$

where k indicates the k th component of the mixture and $\boldsymbol{\phi} = \{\boldsymbol{\pi}, \boldsymbol{\psi}\}$ with $\boldsymbol{\psi} = \{\boldsymbol{\psi}_1, \dots, \boldsymbol{\psi}_K\}$ the mixture parameters. In the EM framework, an additional variable \mathbf{Z} is introduced to identify the missing class labels, where $\{Z_1, \dots, Z_N\}$ define the component of origin of the data $\{\mathbf{y}_1, \dots, \mathbf{y}_N\}$. In the light of the characterization of multiple scaled distributions, an equivalent modelling is: $\forall i \in \{1 \dots N\}$,

$\mathbf{Y}_i | \mathbf{W}_i = \mathbf{w}_i, Z_i = k \sim \mathcal{N}_M(\boldsymbol{\mu}_k + \mathbf{D}_k \boldsymbol{\Delta}_{\mathbf{w}_i} \mathbf{A}_k \mathbf{D}_k^T \boldsymbol{\beta}_k, \mathbf{D}_k \boldsymbol{\Delta}_{\mathbf{w}_i} \mathbf{A}_k \mathbf{D}_k^T)$ and $\mathbf{W}_i | Z_i = k \sim \mathcal{IG}(\gamma_{1k}, \delta_k) \otimes \dots \otimes \mathcal{IG}(\gamma_{Mk}, \delta_k)$, where $\boldsymbol{\Delta}_{\mathbf{w}_i} = \text{diag}(w_{i1}, \dots, w_{iM})$. Inference using the EM algorithm with two sets of missing variables $\mathbf{Z} = \{Z_1, \dots, Z_N\}$ and $\mathbf{W} = \{\mathbf{W}_1, \dots, \mathbf{W}_N\}$ to fit such mixtures, is similar to the individual ML estimation (see Appendix C).

As the results of the EM algorithm can be particularly sensitive to initial values (Karlis and Xekalaki, 2003), for the results to follow we used a number of approaches to generate different initial values for parameters, including the use of random partitions, k -means and trimmed k -means (Garcia-Escudero and Gordaliza, 1999). Often the most successful strategy found was by estimating $\boldsymbol{\mu}_k$, \mathbf{D}_k and

\mathbf{A}_k using the results from a trimmed k -means clustering (with $\beta_k = 0$) and setting $\gamma_{km} = \delta_k = 1$ for all $k = 1 \dots K$ and $m = 1 \dots M$. The computational speed of the EM algorithm for the MSNIG distribution is comparable to the standard NIG case with the exception that the update of \mathbf{D} can be slow for high dimensional applications as the Flury and Gautschi algorithm involves sequentially updating every pair of column vectors of \mathbf{D} . A more global approach to the update of \mathbf{D} has been proposed recently by Browne and McNicholas (2012) which has the potential to significantly speed up the computation time.

4 Applications of multiple scaled NIG distributions

In this section we use simulated data and present applications of the multiple scaled NIG distribution on two real datasets to demonstrate its flexibility in analysing skewed multivariate data.

4.1 Simulated data

For this example, we simulated data from a mixture of MSNIG distributions and assessed the classification performance of the MSNIG compared to the standard NIG. The classification performance of the MSNIG compares favourably to the standard NIG with the MSNIG better able to capture the heavy tails of the two clusters. For details see Appendix A of the Supplementary Materials.

4.2 Petroleum data

This data consists of 655 petroleum samples collected from the Montrose quadrangle of Western Colorado. The samples consist of log-concentration readings for a number of chemical elements, and are part of a multivariate dataset originally described by Cook and Johnson (1981). The dataset is often used to compare and contrast different copula approaches (Genest and Rivest, 1993). For ease of analysis and presentation we concentrate on two of the elements Cobalt (Co) and Uranium (U). Figure 5 provides a scatterplot of the data overlaid with contour lines for the standard NIG (red dashed) and multiple scaled NIG (blue) displayed. From the contour lines we can see that the multiple scaled NIG provides a better fit to the data and this is also evidenced by significantly higher likelihood and BIC estimates for the multiple scaled NIG ($\mathcal{L} = 207.5$, $\text{BIC} = -387$) compared to the standard NIG ($\mathcal{L} = 168.4$, $\text{BIC} = -334$).

4.3 Lymphoma data

To further illustrate some of the differences between the standard NIG and multiple scaled NIG we examine a clustering problem for a lymphoma dataset recently analysed by Lee and McLachlan (2012). The data consists of a subset of data originally presented and collected by Maier et al. (2007). In Maier et al. (2007) blood samples from 30 subjects were stained with four fluorophore-labeled antibodies against $CD4$, $CD45RA$, $SLP76(pY128)$, and $ZAP70(pY292)$ before and after an anti- $CD3$ stimulation. In the first example we will look at

Table 1: Estimated parameters for MSNIG and NIG on the Petroleum data (Co v. U)

Parameters	MSNIG	NIG
μ	(0.96,0.35)	(0.99,0.46)
β	(2.73,13.57)	(2.10,5.25)
D	$\begin{pmatrix} 0.06 & -0.99 \\ 0.99 & 0.06 \end{pmatrix}$	-
A	diag(1.08, 0.93)	-
Σ	-	$\begin{pmatrix} 0.51 & -0.01 \\ -0.01 & 1.97 \end{pmatrix}$
γ	(8.17,14.69)	8.77
δ	0.28	0.33
Log-like	207.6	168.4

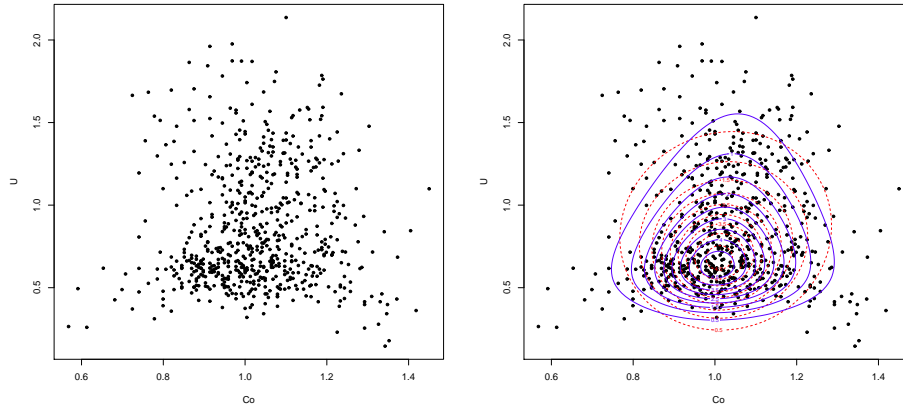


Figure 5: Scatterplot of petroleum data (Co v. U). Right panel: Comparison of standard NIG (red, dashed line) versus MSNIG (blue).

clustering a subset of the data containing the variables $CD4$ and $ZAP70$ (Figure 6), which appear to be bimodal and display an asymmetric pattern. In particular, one of the modes appears to show both strong correlation between the two variables and substantial skewness.

Of interest in this example is to compare the goodness of fit from fitting mixtures of standard NIG and multiple scaled NIG distributions. For comparison, we also present the results of fitting using mixtures of skew-normal (Lachos et al., 2010) and skew- t distributions using two types of formulation: one in which there is some separation between skewness and tail behaviour and referred to as *unrestricted* (Sahu et al., 2003; Lee and McLachlan, 2012; Lin, 2010) and one with no such separation (Azzalini and Dalla Valle, 1996; Basso et al., 2010; Pyne et al., 2009). Estimation of the parameters for these distributions was undertaken using the R package **mixsmsn** (Cabral et al., 2012) and for the unrestricted skew- t case using R code available on: <http://www.maths.uq.edu.au/~gjm/mi>.

Figures 6 (a) to (d) show the separate contour lines (of each component) from fitting mixtures of: standard NIG (Karlis and Santourian, 2009)(a); unrestricted Skew- t (Sahu et al., 2003; Lee and McLachlan, 2012; Lin, 2010) (b); Skew- t (Azzalini and Dalla Valle, 1996; Basso et al., 2010; Pyne et al., 2009) (c); and multiple scaled NIG (d). Likelihood values and estimates of the BIC for the different approaches are also provided in Table 2. As we can see from Figure 6 there is quite a difference in the goodness of fit between the approaches. In particular, we see a clear difference in the fitted results between the standard NIG and multiple scaled NIG with the latter providing a closer fit to the data. Similar results to the standard NIG are obtained for the *no separation* Skew- t (c) and Skew-normal (Lachos et al., 2010) (not shown) approaches. Interestingly the fitted results of the *unrestricted* Skew- t (b) and the multiple scaled NIG (d) appear to be similar. BIC values for these two approaches are also similar (MSNIG = 47,175, *unrestr.* Skew- t = 47,103) but with more support for the *unrestricted* Skew- t .

Table 2: Results for Lymphoma dataset

Model	Example 1 ($CD4$ v. $ZAP70$)		Example 2 ($CD45$ v. $CD4$)	
	Log-likelihood	BIC	Log-likelihood	BIC
MSNIG	-23,545	47,175	-16,444	33,046
NIG	-23,842	47,691	-16,573	33,289
Skew- t (Unrestr.)	-23,492	47,103	-16,540	33,310
Skew- t	-23,868	47,874	-16,561	33,385
Skew-normal	-23,762	47,663	-16,573	33,410

As noted by Lee and McLachlan (2012) a possible reason for the difference in the results between the unrestricted Skew- t (e.g. Sahu et al. (2003)) and the skew-normal and Skew- t (e.g. (Azzalini and Dalla Valle, 1996)) is the differing degree of dependency between the skewness parameter and the covariance for the different approaches. As mentioned previously, in the skew- t formulation of Sahu et al. (2003) there is some separation between the skewness parameter and the covariance, which is not the case for the other formulations of the skew- t

and skew-normal approaches.

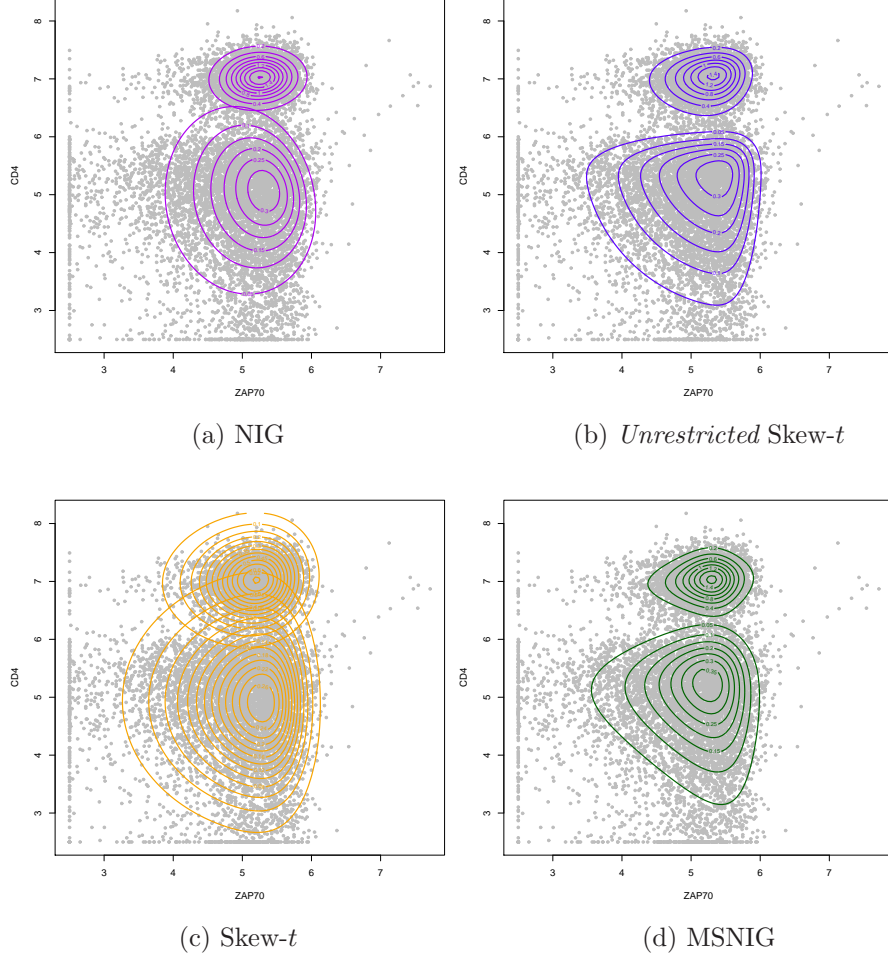


Figure 6: Lymphoma data, $CD4$ v. $ZAP70$. Fitted contour lines for: (a) Standard NIG (Karlis and Santourian, 2009); (b) *Unrestricted Skew-t* (Sahu et al., 2003); (c) *Skew-t* (Azzalini and Dalla Valle, 1996); and (d) Multiple scaled NIG.

We now consider a second example to highlight further differences between the standard NIG and multiple scaled NIG in a clustering context using the same dataset. In this example we look at a subset of the dataset containing the variables $CD45$ and $CD4$, which also appear to be highly multimodal and asymmetric in shape. The fitted results from a mixture model with four components are shown in Figure 7 with contour lines representing the fitted density of each component (see also results in Table 2). From the fitted results we can see a better fit from the multiple scaled NIG ($BIC = 33,046$) compared to the standard NIG ($BIC = 33,289$). The better fit appears to come from the increased flexibility of the multiple scaled NIG to represent non-elliptical shapes. The fitted results for the *Skew-t* and *unrestr.* *Skew-t* do not appear to be better

than for the standard NIG (BIC = 33,385 and 33,310, respectively). Similar results to the Skew- t are found for the Skew-normal (not shown).

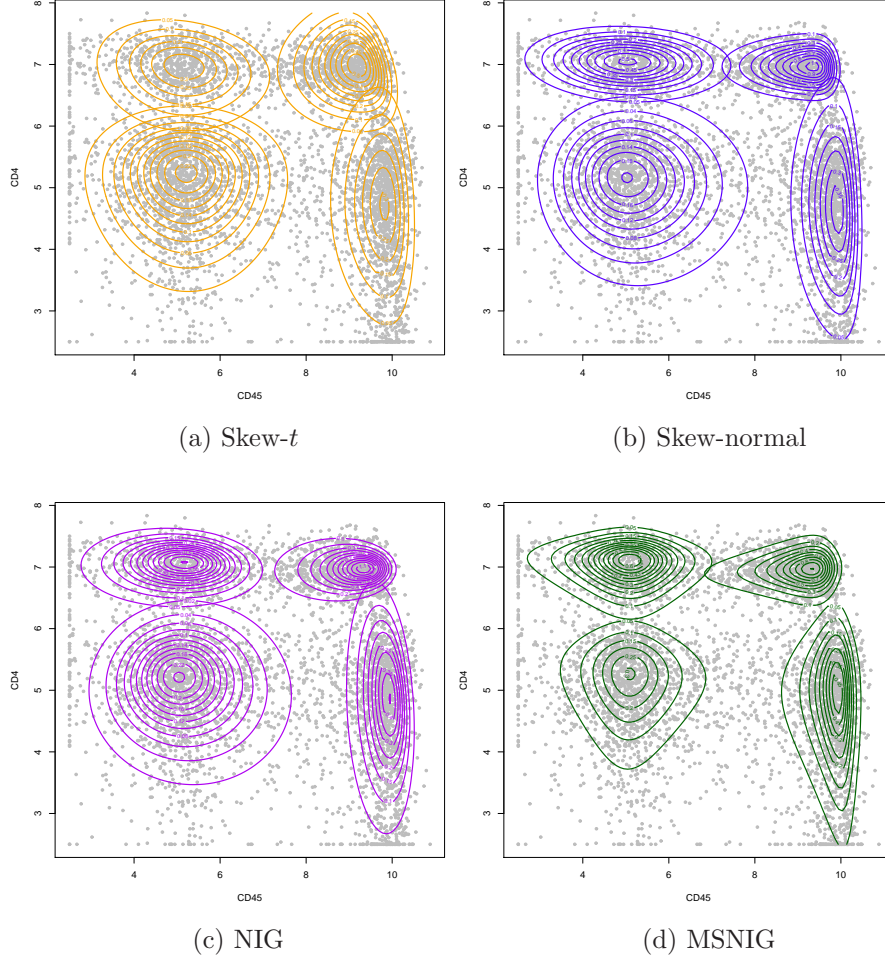


Figure 7: Lymphoma data, $CD45$ v. $CD4$. Fitted contour lines for: (a) Skew- t ; (b) *Unrestricted* Skew- t ; (c) Standard NIG; and (d) Multiple scaled NIG.

5 Conclusion

We have proposed a relatively simple way to extend *location and scale mixture distributions*, such as the multivariate generalised hyperbolic distribution (GH), to allow for different tail behaviour in each dimension. In contrast to existing approaches, the approach has the advantage of: a closed form density; allowing arbitrary correlation between dimensions; and applicability to high dimensional spaces. Estimation of the parameters of the multiple scaled GH (including the important multiple scaled NIG as a particular case) is also relatively straightforward using the familiar EM algorithm and various properties of the family

are well defined. Assessments of the performance of the proposed model on simulated and real data suggest that the extension provides a considerable degree of freedom and flexibility in modelling data of varying tail behaviour and directional shape.

For future research, parsimonious models could be considered using special decompositions of the scale matrix such as in the model-based clustering approach of Celeux and Govaert (1995) and Fraley and Raftery (2002), which would be straightforward to generalize to multiple scaled distributions. Similarly, for very high dimensional data, other parsimonious models could also be considered with a special modelling of the covariance matrix such as in the High Dimensional Data Clustering (HDDC) framework of Bouveyron et al. (2007).

Although we have illustrated the approach on clustering examples, the multiple scaled NIG is applicable to other contexts including, for example, regression modelling, outlier detection and modelling of spatial data (Forbes et al., 2010).

Appendices

Appendix A: Multiple Scaled Normal Inverse Gaussian distribution (MSNIG)

In the case of the MSNIG where $W_m \sim \mathcal{IG}(\lambda_m = -1/2, \gamma_m, \delta_m)$, expressions (16) and (17) simplify into

$$\begin{aligned} E[\mathbf{Y}_{MSNIG}] &= \boldsymbol{\mu} + \mathbf{D}E[\Delta_W]\mathbf{A}\mathbf{D}^T\boldsymbol{\beta} \\ &= \boldsymbol{\mu} + \mathbf{D}\text{diag}\left(\frac{\delta_1}{\gamma_1}, \dots, \frac{\delta_M}{\gamma_M}\right)\mathbf{A}\mathbf{D}^T\boldsymbol{\beta} \end{aligned} \quad (36)$$

$$\text{Var}[\mathbf{Y}_{MSNIG}] = \mathbf{D}\text{diag}\left(\frac{\delta_1}{\gamma_1}, \dots, \frac{\delta_M}{\gamma_M}\right)\mathbf{A}\mathbf{D}^T \quad (37)$$

$$\begin{aligned} &+ \mathbf{D}\text{diag}\left(\frac{\delta_1}{\gamma_1^3}[\mathbf{D}^T\boldsymbol{\beta}]_1^2, \dots, \frac{\delta_M}{\gamma_M^3}[\mathbf{D}^T\boldsymbol{\beta}]_M^2\right)\mathbf{A}\mathbf{D}^T \\ &= \mathbf{D}\text{diag}\left(\frac{\delta_m A_m}{\gamma_m}\right)\left(1 + \frac{[\mathbf{D}^T\boldsymbol{\beta}]_m^2 A_m}{\gamma_m^2}\right)\mathbf{D}^T \end{aligned} \quad (38)$$

Appendix B: Algorithm for computing $D^{(r+1)}$

The goal is to minimize with respect to D the following quantity, where \tilde{A} , μ and $\tilde{\beta}$ have been fixed to current estimations namely $\tilde{A}^{(r)}$, $\mu^{(r+1)}$ and $\tilde{\beta}^{(r+1)}$,

$$D^{(r+1)} = \arg \min_D f(D)$$

$$\begin{aligned} \text{where } f(D) = & \sum_{i=1}^N \text{trace}(D T_i^{(r)} \tilde{A}^{-1(r)} D^T V_i) + \sum_{i=1}^N \text{trace}(D S_i^{(r)} \tilde{A}^{-1(r)} D^T B_i) \\ & - 2 \left(\sum_{i=1}^N \text{trace}(D \tilde{A}^{-1} D^T C_i) \right) \end{aligned}$$

where $V_i = (\mathbf{y}_i - \mu^{(r+1)})(\mathbf{y}_i - \mu^{(r+1)})^T$, $B_i = \tilde{\beta}^{(r+1)} \tilde{\beta}^{T(r+1)}$, $C_i = (\mathbf{y}_i - \mu^{(r+1)}) \tilde{\beta}^{T(r+1)}$. Similarly to Celeux and Govaert (1995, see Appendix 2), we can derive from Flury and Gautschi (1986) the algorithm below.

Step 1. We start from an initial solution $D^0 = [\mathbf{d}_1^0, \dots, \mathbf{d}_M^0]$ where the \mathbf{d}_m^0 's are M -dimensional orthonormal vectors.

Step 2. For any couple $(l, m) \in \{1, \dots, M\}^2$ with $l \neq m$, the couple of vectors $(\mathbf{d}_l, \mathbf{d}_m)$ is replaced with $(\boldsymbol{\delta}_l, \boldsymbol{\delta}_m)$ where $\boldsymbol{\delta}_l = [\mathbf{d}_l, \mathbf{d}_m] \mathbf{v}_1$ and $\boldsymbol{\delta}_m = [\mathbf{d}_l, \mathbf{d}_m] \mathbf{v}_2$ with \mathbf{v}_1 and \mathbf{v}_2 two orthonormal vectors of \mathbb{R}^2 such that \mathbf{v}_1 is the eigenvector associated to the smallest eigenvalue of the matrix

$$\begin{aligned} M = & \sum_{i=1}^N \left(\frac{t_{il}^{(r)}}{A_l^{(r)}} - \frac{t_{im}^{(r)}}{A_m^{(r)}} \right) [d_l, d_m]^T V_i [d_l, d_m] + \sum_{i=1}^N \left(\frac{s_{il}^{(r)}}{A_l^{(r)}} - \frac{s_{im}^{(r)}}{A_m^{(r)}} \right) [d_l, d_m]^T B_i [d_l, d_m] \\ & - 2 \sum_{i=1}^N \left(\frac{1}{A_l^{(r)}} - \frac{1}{A_m^{(r)}} \right) [d_l, d_m]^T C_i [d_l, d_m] \end{aligned}$$

Step 2 is repeated until it produces no decrease of the criterion $f(D)$.

Appendix C: Mixture setting and estimation

Denote the parameters of the mixture in the equivalent parameterization (26) by $\phi = \{\pi, \tilde{\psi}\}$ with $\tilde{\psi} = \{\tilde{\psi}_1, \dots, \tilde{\psi}_K\}$ the mixture parameters with $\tilde{\psi}_k = \{\mu_k, \mathbf{D}_k, \tilde{\mathbf{A}}_k, \tilde{\beta}_k, \tilde{\gamma}_k\}$ for $k = 1 \dots K$. For mixtures the EM algorithm iterates over the following two steps.

E-step

We denote by $\tau_{ik}^{(r)}$ the posterior probability that \mathbf{y}_i belongs to the k th component of the mixture given the current estimates of the mixture parameters $\phi^{(r)}$,

$$\tau_{ik}^{(r)} = \frac{\pi_k^{(r)} \mathcal{MSNIG}(\mathbf{y}_i; \psi_k^{(r)})}{p(\mathbf{y}; \phi^{(r)})} \quad (39)$$

The conditional expectation of the complete data log-likelihood $Q(\phi, \phi^{(r)})$ decomposes into three parts

$$Q(\phi, \phi^{(r)}) = Q_1(\pi; \phi^{(r)}) + Q_2(\tilde{\gamma}; \phi^{(r)}) + Q_3(\mu, \mathbf{D}, \tilde{\mathbf{A}}, \tilde{\beta}, \tilde{\gamma}; \phi^{(r)}) \quad (40)$$

with

$$Q_1(\pi; \phi^{(r)}) = \sum_{i=1}^N \sum_{k=1}^K \tau_{ik}^{(r)} \log \pi_k \quad (41)$$

$$Q_2(\tilde{\gamma}; \phi^{(r)}) = \sum_{i=1}^N \sum_{k=1}^K \tau_{ik}^{(r)} \sum_{m=1}^M E_{W_{im}} [\log \mathcal{IG}(W_{im}; \tilde{\gamma}_{km}, 1) | \mathbf{y}_i, \phi^{(r)}] \quad (42)$$

and

$$\begin{aligned} Q_3(\tilde{\gamma}; \phi^{(r)}) &= \sum_{i=1}^N \sum_{k=1}^K \tau_{ik}^{(r)} E_{W_i} [\log \mathcal{N}(\mu_k + \\ &\quad \mathbf{D}_k \Delta_{\mathbf{w}_i} \tilde{\mathbf{A}}_k \mathbf{D}_k^T \tilde{\beta}_k, \mathbf{D}_k \Delta_{\mathbf{w}_i} \tilde{\mathbf{A}}_k \mathbf{D}_k^T) | Z_i = k, \mathbf{y}_i, \phi^{(r)}] \\ &= \sum_{i=1}^N \sum_{k=1}^K \tau_{ik}^{(r)} E_{W_i} [-\frac{1}{2} (\mathbf{y}_i - \mu_k - \mathbf{D}_k \Delta_{\mathbf{w}_i} \mathbf{D}_k^T \tilde{\beta}_k)^T \mathbf{D}_k \tilde{\mathbf{A}}^{-1} \Delta_{\mathbf{w}_i}^T \mathbf{D}_k^T \\ &\quad \times (\mathbf{y}_i - \mu_k - \mathbf{D}_k \Delta_{\mathbf{w}_i} \mathbf{D}_k^T \tilde{\beta}_k) | Z_i = k, \mathbf{y}_i, \phi^{(r)}] - \frac{1}{2} \log |\tilde{\mathbf{A}}_k| \end{aligned} \quad (43)$$

ignoring constants.

Similarly to the E-step in Section 3.1, the quantities required for the E-step are given by,

$$\begin{aligned} s_{ikm}^{(r)} &= E[W_{im} | Z_i = k, \mathbf{y}_i; \phi^{(r)}] = \frac{\phi_{ikm}^{(r)} K_0(\phi_{ikm}^{(r)} \hat{\alpha}_{km}^{(r)})}{\hat{\alpha}_{km}^{(r)} K_{-1}(\phi_{ikm}^{(r)} \hat{\alpha}_{km}^{(r)})} \\ t_{ikm}^{(r)} &= E[W_{im}^{-1} | Z_i = k, \mathbf{y}_i; \phi^{(r)}] = \frac{\hat{\alpha}_{km}^{(r)} K_{-2}(\phi_{ikm}^{(r)} \hat{\alpha}_{km}^{(r)})}{\phi_{ikm}^{(r)} K_{-1}(\phi_{ikm}^{(r)} \hat{\alpha}_{km}^{(r)})} \end{aligned}$$

where

$$\begin{aligned}\phi_{ikm}^{(r)} &= \sqrt{1 + \frac{[\mathbf{D}_k^{(r)T}(\mathbf{y}_i - \boldsymbol{\mu}_k^{(r)})]_m^2}{\tilde{\mathbf{A}}_{km}^{(r)}}} \\ \hat{\alpha}_{km}^{(r)} &= \sqrt{\tilde{\gamma}_{km}^{2(r)} + \frac{[\mathbf{D}_k^{(r)T}\tilde{\boldsymbol{\beta}}_k^{(r)}]_m^2}{\tilde{\mathbf{A}}_{km}^{(r)}}}\end{aligned}$$

M-step

Updating the π_k 's. The update of $\boldsymbol{\pi}$ is standard: for $k \in \{1, \dots, K\}$, $\pi_k^{(r+1)} = \frac{n_k}{N}$ where $n_k = \sum_{i=1}^N \tau_{ik}^{(r)}$.

Updating the $\boldsymbol{\mu}_k$'s. It follows from the expression of Q_3 that for $k \in \{1, \dots, K\}$, fixing \mathbf{D}_k to the current estimation $\mathbf{D}_k^{(r)}$, leads for all $m = 1, \dots, M$ to

$$\begin{aligned}\boldsymbol{\mu}_{km}^{(r+1)} &= \left(\frac{\sum_{i=1}^N \tau_{ik} \mathbf{T}_{ik}^{(r)} \mathbf{D}_k^{(r)T}}{n_k} - n_k \left(\sum_{i=1}^N \tau_{ik} \mathbf{S}_{ik}^{(r)} \right)^{-1} \right)^{-1} \\ &\quad \left(\frac{\sum_{i=1}^N \tau_{ik} \mathbf{T}_{ik}^{(r)} \mathbf{D}_k^{(r)T} \mathbf{y}_i}{n_k} - \sum_{i=1}^N \tau_{ik} \mathbf{y}_i \left(\sum_{i=1}^N \tau_{ik} \mathbf{S}_{ik}^{(r)} \right)^{-1} \right)\end{aligned}$$

where $\mathbf{T}_{ik}^{(r)} = \text{diag}(t_{ik1}^{(r)}, \dots, t_{ikM}^{(r)})$ and $\mathbf{S}_{ik}^{(r)} = \text{diag}(s_{ik1}^{(r)}, \dots, s_{ikM}^{(r)})$.

Updating the $\tilde{\boldsymbol{\beta}}_k$'s. Similarly, it follows from the expression of Q_3 that for $k \in \{1, \dots, K\}$, fixing \mathbf{D}_k and $\boldsymbol{\mu}_k$ to their current estimation $\mathbf{D}_k^{(r)}$ and $\boldsymbol{\mu}_k^{(r)}$, leads to

$$\tilde{\boldsymbol{\beta}}_k^{(r+1)} = \mathbf{D}_k^{(r)} \left(\sum_{i=1}^N \tau_{ik}^{(r)} \mathbf{S}_{ik}^{(r)} \right)^{-1} \mathbf{D}_k^{(r)T} \sum_{i=1}^N \tau_{ik}^{(r)} (\mathbf{y}_i - \boldsymbol{\mu}_k^{(r+1)})$$

Updating the \mathbf{D}_k 's

The parameter \mathbf{D}_k is obtained by minimizing

$$\begin{aligned}\mathbf{D}_k^{(r+1)} &= \arg \min_{\mathbf{D}_k} \left(\sum_{i=1}^N \text{trace}(\mathbf{D}_k \mathbf{T}_{ik}^{(r)} \tilde{\mathbf{A}}_k^{(r)-1} \mathbf{D}_k^T \mathbf{V}_{ik}) \right. \\ &\quad \left. + \sum_{i=1}^N \text{trace}(\mathbf{D}_k \mathbf{S}_{ik}^{(r)} \tilde{\mathbf{A}}_k^{(r)-1} \mathbf{D}_k^T \mathbf{B}_{ik}) - 2 \left(\sum_{i=1}^N \text{trace}(\mathbf{D}_k \tilde{\mathbf{A}}_k^{(r)-1} \mathbf{D}_k^T \mathbf{C}_{ik}) \right) \right)\end{aligned}$$

where $\mathbf{V}_{ik} = \tau_{ik}^{(r)} (\mathbf{y}_i - \boldsymbol{\mu}_k^{(r+1)}) (\mathbf{y}_i - \boldsymbol{\mu}_k^{(r+1)})^T$, $\mathbf{B}_{ik} = \tau_{ik}^{(r)} \tilde{\boldsymbol{\beta}}_k^{(r+1)} \tilde{\boldsymbol{\beta}}_k^{(r+1)T}$ and $\mathbf{C}_{ik} = \tau_{ik}^{(r)} (\mathbf{y}_i - \boldsymbol{\mu}_k^{(r+1)}) \tilde{\boldsymbol{\beta}}_k^{(r+1)T}$.

The parameter \mathbf{D}_k can be updated using an algorithm derived from Flury and Gautschi (see Flury and Gautschi, 1986, and Appendix B).

Updating the $\tilde{\mathbf{A}}_k$'s. We have to minimize the following quantity:

$$\tilde{\mathbf{A}}_k^{(r+1)} = \arg \min_{\tilde{\mathbf{A}}_k} \left(\text{trace} \left(\sum_{i=1}^N \mathbf{M}_{ik} \tilde{\mathbf{A}}_k^{-1} \right) + \alpha_k \log |\tilde{\mathbf{A}}_k| \right)$$

where $M_{ik} = \mathbf{T}_{ik}^{(r)1/2} \mathbf{D}_k^{(r+1)T} \mathbf{V}_{ik} \mathbf{D}_k^{(r+1)} \mathbf{T}_{ik}^{(r)1/2} + \mathbf{S}_{ik}^{(r)1/2} \mathbf{D}_k^{(r+1)T} \mathbf{B}_{ik} \mathbf{D}_k^{(r+1)} \mathbf{S}_{ik}^{(r)1/2} - \mathbf{D}_k^{(r+1)T} (\mathbf{C}_{ik} + \mathbf{C}_{ik}^T) \mathbf{D}_k^{(r+1)}$ is a symmetric positive definite matrix and $\alpha_k = \sum_{i=1}^N \tau_{ik}^{(r)}$

Using Corollary 3.2 (see Section 3) leads for all $m = 1, \dots, M$ to

$$\begin{aligned} \tilde{\mathbf{A}}_{km}^{(r+1)} = & \frac{1}{\sum_{i=1}^N \tau_{ik}^{(r)}} \sum_{i=1}^N \tau_{ik}^{(r)} \left([\mathbf{D}_k^{(r+1)T} (\mathbf{y}_i - \boldsymbol{\mu}_k^{(r+1)})]_m^2 t_{ikm}^{(r)} + [\mathbf{D}_k^{(r+1)T} \tilde{\boldsymbol{\beta}}_k^{(r+1)}]_m^2 s_{ikm}^{(r)} \right. \\ & \left. - 2[\mathbf{D}_k^{(r+1)T} (\mathbf{y}_i - \boldsymbol{\mu}_k^{(r+1)})]_m [\mathbf{D}_k^{(r+1)T} \tilde{\boldsymbol{\beta}}_k^{(r+1)}]_m \right) \end{aligned}$$

Updating the $\tilde{\gamma}_k$'s. To update $\tilde{\gamma}_k$ we have to minimize,

$$\tilde{\gamma}_k^{(r+1)} = \arg \min_{\tilde{\gamma}} \left\{ \sum_{i=1}^N \tau_{ik}^{(r)} \sum_{m=1}^M \frac{1}{2} \tilde{\gamma}_{km}^2 s_{ikm}^{(r)} - \tilde{\gamma}_{km} \right\}$$

which leads for all $m = 1, \dots, M$ to

$$\tilde{\gamma}_{km}^{(r+1)} = \frac{n_k}{\sum_{i=1}^N \tau_{ik} s_{ikm}}$$

To transform the estimated parameters back to the original ones, $\delta_k = |\tilde{\mathbf{A}}_k|^{\frac{1}{2M}}$, $\gamma_{km} = \tilde{\gamma}_{km} / \delta_k$, $\beta_k = \mathbf{D}_k \tilde{\mathbf{A}}_k^{-1} \mathbf{D}_k^T \tilde{\boldsymbol{\beta}}_k$, $\mathbf{A}_k = \tilde{\mathbf{A}}_k / |\tilde{\mathbf{A}}_k|^{\frac{1}{M}}$

Appendix D: Tail dependence

Using Coles et al. (1999) and the R package ‘evd’ (Team, 2011), we assume that the data are *i.i.d.* random vectors with common bivariate distribution function G , and we define the random vector $[X, Y]^T$ to be distributed according to G .

The $\chi(q)$ plot is a plot of q in $(0, 1)$ (interpreted as a quantile level) against empirical estimates of function

$$\chi(q) = 2 - \log(p(F_X(X) < q, F_Y(Y) < q)) / \log(q) \quad (44)$$

where F_X and F_Y are the marginal distribution functions. The quantity $\chi(q)$ is bounded by

$$2 - \log(2q - 1) / \log(q) \leq \chi(q) \leq 1$$

where the lower bound is interpreted as $-\infty$ for $q \leq 1/2$ and zero for $q = 1$.

The function $\chi(q)$ can be interpreted as a quantile dependent measure of dependence. In particular, the sign of $\chi(q)$ determines whether the variables are positively or negatively associated at quantile level q .

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